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Identification and Initial Evaluation of Irrigation Return Flow Models

Irrigation Hydrology Co, Fort Collins, CO

Prepared for

Robert S Kerr Environmental Research Lab, Ada, OK Source Management Branch

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Robert S. Kerr Environmental Research
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Ada OK 74820

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IRF modeling technology is well developed theoretically but not completely verified due to the large scale of the irrigation system. Most models remain in the research sphere and need to be redefined for the wider utilization of planners. Field data are generally not available to satisfy the input requirements of most IRF models. Accuracies of predictions need to be determined against standardized conditions in order to further model development and parameter sensitivities should be investigated to isolate the most important field data.

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IDENTIFICATION AND INITIAL EVALUATION OF IRRIGATION RETURN FLOW MODELS

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FOREWORD

The Environmental Protection Agency was established to coordinate administration of the major Federal programs designed to protect the quality of our environment.

An important part of the Agency's effort involves the search for information about environmental problems, management techniques and new technologies through which optimum use of the Nation's land and water resources can be assured and the threat pollution poses to the welfare of the American people can be minimized.

EPA's Office of Research and Development conducts this search through a nationwide network of research facilities.

As one of these facilities, the Robert S. Kerr Environmental Research Laboratory is responsible for the management of programs to: (a) investigate the nature, transport, fate and management of pollutants in groundwater; (b) develop and demonstrate methods for treating wastewaters with soil and other natural systems; (c) develop and demonstrate pollution control technologies for irrigation return flows; (d) develop and demonstrate pollution control technologies for animal production wastes; (e) develop and demonstrate technologies to prevent, control or abate pollution from the petroleum refining and petrochemical industries; and (f) develop and demonstrate technologies to manage pollution resulting from combinations of industrial wastewaters or industrial/municipal wastewaters.

This report contributes to the knowledge essential if the EPA is to meet the requirements of environmental laws that it establish and enforce pollution control standards which are reasonable, cost effective and provide adequate protection for the American public.

William C Galegar

William C. Galegar
Director
Robert S. Kerr Environmental
Research Laboratory

ABSTRACT

A broad based literature review was undertaken to identify studies that had yielded digital computer models applicable to irrigation return flow (IRF) systems. The programs not listed in technical reports or papers were requested from the various authors. The results of this work are 43 computer models applicable all or in part to the analysis of IRF's and their quality. A brief evaluation of each model is given.

IRF modeling technology is well developed theoretically but not completely verified due to the large scale of the irrigation system. Most models remain in the research sphere and need to be redefined for the wider utilization of planners. Field data are generally not available to satisfy the input requirements of most IRF models. Accuracies of predictions need to be determined against standardized conditions in order to further model development and parameter sensitivities should be investigated to isolate the most important field data.

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SECTION 1

INTRODUCTION

The use of computers in the study of the complex irrigation system processes has provided a means for their rapid and intensive evaluation. The basis for the computer codes (or models) is the expression of the real system as concise mathematical relationships. The transformation between the physical and mathematical forms has been achieved to various degress of success depending on the expertise of the modeler, the objectives and funding of the study, the required time and spatial scales of the investigation, and the availability of data. The major thrust of most models dealing with irrigated agriculture has been associated with the excess water being applied to croplands. The volume of irrigation water needed to promote high crop yields is almost universally less than the volumes diverted for these purposes. Studies have been made to accurately determine the crop evapotranspiration so that irrigation systems could be properly designed and operated. The excess moisture moving through the root zone has been investigated in many respects, some of which include salt and fertilizer leaching and drainage requirements. The quality of the irrigation wastewater (called irrigation return flows, IRF) has been of primary concern in recent years as efforts have been made to maintain suitable water quality in all water resources.

The principal interest of this work is the digital computer models which deal with the environmental impact of irrigation return flows. These are the models which simulate the occurrence and magnitude of the flows, their quality characteristics, and their effects on receiving waters. Recognizing that the IRF system is an aggregate of several complex hydrologic, chemical, and biological processes, this group of models also includes simulations of the basic processes. The objective of this project was to identify and initially evaluate available IRF computer programs. The evaluation is intended to be somewhat general, including a brief description of the model scope, input requirements, characteristics of the computer code, expected time and spatial resolutions, basic mathematical approach, and if possible a note concerning previous applications, calibration, or verification.

There is an underlying intent that these IRF models become more widely utilized. A substantial duplication of effort is evident in the formulation and testing phases of various models, but this may be a minor problem compared with the dissemination of the models to what might be called the "applied users" (planners, consultants, government agency personnel, etc.). Most IRF models originate as research tools used to investigate the basic behavior of irrigated agriculture. Research interests seek an understanding of the various hydro-quality mechanisms and their interactions enroute to identifying the effectiveness of alternative management measures. The research modeler attempts to simulate as much real system detail as is possible. Output is generally related to the time and spatial distribution of parameters, and is generally compared to specially collected field data to validate the approach and its assumptions. Both time and spatial resolutions are small (many models study processes in a single vertical profile in terms of minutes and extending no more than the period between irrigations).

In contrast, there is a large number of people not so much interested in understanding the problem as they are in getting it alleviated. These are the personnel charged with providing support to decision makers and administrators who recommend remedies or implementation policies to funding agencies and legislatures. Their view of the problem tends to be very macroscopic, i.e., problems with inadequate field data for finely tuned research models, a system of thousands or millions of hectares and time frames of months and years.

This study was organized to make an initial assessment of the existing IRF modeling capability with a view towards improving the availability of the programs for use by others. In order that the reader might better understand the selection of models, as will be discussed in later sections, several points concerning the scope of the study should be made. The models evaluated in this report were identified from an intensive review of the technical literature. A large number of "models" are entirely mathematical or conceptual, and are therefore not included. Some models appear in the literature under different authors and applied to different situations. For this study, only the most recent or more complete version is included. There appear to be both studies in which a computer code is developed for general use and those in which a program was written only for the purpose of the specific project. These latter models are not generally available for widespread use because documentation has been omitted. These programs which would be difficult to use simply because no documentation is available or because of rough coding are not part of this study. It should also be noted that not all models are actually available in the literature and many must be requested from the authors.

This report details some 43 individual models although the actual number represented is much higher. In addition to models having more than one version or revision, some models are combinations of more specific models or subroutines that may, in fact, often be utilized separately. In this work, the most integrated form of the models is presented.

There are several major groundwater model collection and evaluation efforts underway which are similar to this investigation. To avoid duplicating these efforts, groundwater models as such are not included herein.

SECTION 2

CONCLUSIONS

1. The irrigation return flow system and many of its basic elements are well simulated with the existing body of computer models. However, the number of individual models and their differences suggest that modeling advances are not rapidly disseminated, particularly among related fields of interest. Except for some large scale watershed or river basin simulations, few of the IRF models require large core and execution time commitments.

2. All of the programs evaluated were coded in either FORTRAN or CSMP. Both languages have advantages to their users: time and core requirements are smaller for FORTRAN programs; programming is simpler and faster with CSMP. Many computers, particularly those other than IBM machines, will not accommodate CSMP thereby limiting the widespread use of these programs. FORTRAN versions are universally applicable.

3. Examination of the computer codes reveals a wide range of skills in manipulating data, ordering calculations, and preparing output. Models using tape or disc drives are more difficult to apply on other computers because of more variability in the format of these operations. Card input is widely used and offers little or no restrictions. Few programs present output data in an orderly and clear way. In fact, many simply dump numbers without any labeling.

4. The principal element in modeling any IRF system is the region from the crop canopy to the water table. This subgroup of IRF models is the best developed and tested. Unfortunately, available field data are insufficient for most of these models so they are primarily research tools. One of the most severe data deficiencies is the description of the soil hydraulic properties, i.e., hydraulic conductivity as a function of moisture content, and moisture content as a function of soil moisture potential. If these data are known, however, soil moisture flux is readily simulated. The nitrogen cycle remains the most elusive quality component of the unsaturated zone hydrology primarily because it is an organic, biological series of transformations. Evapotranspiration is a well modeled process when estimates are based on climatological data. Separation of transpiration and evaporation as well as predicting the distribution of root water extraction is less developed.

5. Other subsets of the IRF models examined are also primarily slanted toward research rather than planning applications. Most if not all also require at least some input data not generally available. Consequently, there is not an IRF modeling capability for evaluation of large scale irrigated agriculture which can be utilized by the various nonresearch

professionals. This is a serious problem because it prevents an accurate assessment of the effectiveness of alternative measures for managing the quality of irrigation return flows.

6. Most models are written to be more general than actually required in their initial use. Consequently, there are often completely untested loops within these programs. Another user with a different set of conditions may find problems in these heretofore unused loops. There needs to be at least two or more sets of data to serve as "standards" for the testing, evaluation, and comparison of IRF models.

7. Although the models discussed in this report focus on the subject of IRF quality, they are also valuable tools in other investigations. The basic processes simulated also provide the means for evaluating such topics as energy conservation and storage in agricultural systems, maximizing yields under drought conditions, disposal and impacts of organic wastes in agricultural soils, and the feasibility of alternative irrigation systems.

SECTION 3

RECOMMENDATIONS

1. A library of the models identified in this study and others as they become available should be organized at a central resource point for a wider dissemination. The library should include operational programs, a detailed documentation for each model, and an example calculation. Provisions should be made for periodic updating of the models and the acquisition of newly developed programs.

2. There are many duplicative models. Thus, each phase of the IRF modeling technology should be condensed. The relevant expertise should be brought together with the purpose of developing a "second generation" series of models by taking the best parts from all available models and producing a series of models incorporating the strongest features of the existing technology.

3. The CSMP models should be rewritten in FORTRAN for wider application on other computer systems.

4. The research modelers need to determine the impact of variability in their models. Sensitivities to input data, assumptions, and individual parameters should be evaluated to delineate the kinds of information having the highest priority and the limitations of some mathematical approaches. These analyses need to be made in a comparative format. The sensitivity studies need to occur within the same set of conditions so that effect of different modeling approaches can be ascertained.

5. Recommendation 4 requires two or more detailed data sets. Because of the high cost of field data collection, the available models need to be subdivided and assessed one group at a time. The first priority should be given to the unsaturated zone models. Some data describing this system may be already available. Consideration might also be given to a few completely synthesized data sets representing conditions often encountered in field situations.

6. This largely research-oriented, modeling technology should be redesigned for the much larger need involved in large scale planning studies. Detailed models will probably not be applicable, but should be used to test the larger scope models for their accuracy, dependability, and limitations. Results of this kind of investigation should be utilized to aid basic data collection efforts by detailing the most important data requirements and the priority among types of data.

7. Although there remain a number of modeling deficiencies, none represent serious problems so far as irrigation return flow quality is concerned. A large enough basic research program is continuously operating to remedy these deficiencies in a short time if reporting the respective models can be encouraged. The IRF models need to be visible enough to be utilized in these new research activities so they will be subject to improvement and expansion.

SECTION 4

METHODOLOGY AND RESULTS

MODEL IDENTIFICATION

This project has taken a broad view of what constitutes an "irrigation return flow model." Actually, many of the computer programs were developed for evaluation of individual or combined hydro-quality processes in irrigated agriculture for entirely different objectives, but they are applicable to studies which address the problems of IRF's. Consequently, the models assembled for this report are collectively denoted as IRF models because they are usable and effective. Another study concerned with crop production may just as well refer to some of these same models as "production models" because the same information is necessary.

In recent years, several literature abstracting efforts have been made to identify the pertinent irrigation return flow quality literature (Utah State University Foundation (1969) and Skogerboe et al. (1972, 1973, 1974, 1976, 1977, 1978)). These references served as the initial starting point for this study. Key word indices were searched for such topics as computers, computer models, models, numerical solutions, etc., which would delineate reports where computer models had been developed or utilized. Each potential entry was obtained and evaluated in detail. References cited in these reports which indicated by their titles the further possibilities of model development were also collected and reviewed. This process was repeated until no new literature on the subject of irrigation system models was discovered. Even then, personal contacts with colleagues revealed additional modeling studies. In addition, some literature entirely outside of agriculture was identified in which models applicable to this subject were being generated and used. The final list of references dealing with the fairly narrow topic of modeling totaled more than 200 citations.

The principal interest of this project was digital computer program or code models that might be useful in investigating IRF systems. Models which are conceptual, completely mathematical, physical, or analog are omitted. Many models are listed in reports and papers for the benefit of the potential user and many are left to those sufficiently interested to request copies. There is also a large body of models which are unavailable because they were written for a specific purpose, not generalized to handle alternative forms of the problem, and not documented or prepared for outside use. Many of these fortunately simulate what will be described later as process level systems and are included in other models.

After sifting the literature, the models requiring individual requests were sought. Letters were sent or telephone contacts were made with the individual modelers asking for computer listings and available documentation. Originally, an evaluation questionnaire was planned so that individual modelers could describe their models for this work, but existing Federal regulations prohibited this approach without special approval. Response to the written requests was generally poor.

In earlier work, Walker (1976) concluded that a great deal of model duplication had occurred and that more effort to publicize various modeling efforts would reduce this inefficient use of time and funding. Later in this section this conclusion will be supported. However, in reviewing the literature there are several models which have been used by numerous other researchers. Some models have undergone several revisions and updates, or have been slightly modified for another application. The models referenced in this report are generally the latest version, most complete, most applied, or the ones most available.

The models included herein do not represent an exhaustive listing since there are undoubtedly models which this effort simply did not identify. Nevertheless, the 43 models presented in the appendices encompass much of the technology and certainly many of the best and most verified models available.

MODEL CLASSIFICATION

In summarizing the models assembled for this study it is necessary to segregate the programs into groups having similar scope and purpose. To this end, three major groups of two subclasses each were delineated:

(1) process level models
    (a) infiltration-redistribution
    (b) unsaturated soil solute chemistry and transport

(2) subsystem level models
    (a) unsaturated zone hydrology
    (b) unsaturated zone hydro-quality

(3) system level models
    (a) watershed hydrology
    (b) watershed hydro-quality

Following the subclass designations, the models are described in Appendices A, B, C, D, E, and F. A summary of the various models by major group is given in Tables 1, 2, and 3. In order to present the models more concisely and to illustrate them more nearly as one would expect to use them in modeling IRF systems, the models have been presented in their most aggregated form. The model by Shaffer, et al. (1977), for example, is presented as a single system model even though it consists of seven individual subsystem level models very much usable by themselves.

TABLE 1. CLASSIFICATION OF IRRIGATION RETURN FLOW MODELS AT THE PROCESS LEVEL

REFERENCE	INFILTRATION-REDISTRIBUTION (Appendix A)	UNSATURATED SOIL SOLUTE CHEMISTRY AND TRANSPORT (Appendix B)
Bhuiyan, et al. (1971)	A-1	
Brandt, et al. (1971)	A-2	
Hillel (1977)	A-3	
Lomen and Warrick (1974)	A-4	
Van Der Ploeg and Benecke (1974)	A-5	
Warrick (1974)	A-6	
Warrick and Lomen (1976)	A-7, A-8	
Wind and Van Doorne (1975)	A-9	
Dugard and Reeves (1976)		B-1
Jurinak, et al. (1973)		B-2
Oster and McNeal (1971)		B-3
Rai and Franklin (1973)		B-4
Saxton, et al. (1977)		B-5
Tanji, et al. (1972)		B-6

TABLE 2. CLASSIFICATION OF IRRIGATION RETURN FLOW MODELS AT THE SUBSYSTEM LEVEL

REFERENCE	UNSATURATED ZONE HYDROLOGY (Appendix C)	UNSATURATED ZONE HYDRO-QUALITY (Appendix D)
Feddes and Zaraday (1977)	C-1	
Gupta, et al. (1977)	C-2	
Hillel (1977)	C-3, C-4	D-10
Saxton, et al. (1974)	C-5	
Trava (1975)	C-6	
Neuman, et al. (1975)	C-7	
Beek and Frissel (1973)		D-1
Davidson, et al. (1975)		D-2, D-3
Davidson, et al. (1977)		D-4
DeWit and Van Keulen (1975)		D-5
Frissel and Reiniger (1974)		D-6, D-7, D-8
Hagin and Amberger (1974)		D-9
Margheim (1967)		D-11
Melamed, et al. (1977)		D-12
Smajstrla, et al. (1974)		D-13

TABLE 3. CLASSIFICATION OF IRRIGATION RETURN FLOW MODELS AT THE SYSTEM LEVEL

REFERENCE	WATERSHED HYDROLOGY (Appendix E)	WATERSHED HYDRO-QUALITY (Appendix F)
Hillel (1977)	E-1	
Makkink and Van Heemst (1975)	E-2	
Shaffer, et al. (1977)		F-1
Bureau of Reclamation (1977)		F-2
Crawford and Donigian (1973)		F-3
Dixon, et al. (1970)		F-4
Hill, et al. (1973)		F-5
Walker (1970)		F-6

Process Level Models

The principal hydrologic processes in an irrigation return flow system, illustrated in Figure 1, include transpiration, evaporation, infiltration-redistribution, and root extraction. Associated with each of these processes are a number of chemical and biological transformations affecting the dissolved and adsorbed constituents in the soil. The programs selected for this report which might be classed as process level models are of two types: (1) infiltration-redistribution; and (2) unsaturated soil solute chemistry and transport. Other contributions to irrigation return flows which might be categorized as process level topics, namely irrigation uniformity, conveyance seepage, and field tailwater, are generally not modeled independently. Irrigation uniformity has been recognized recently as an important input to IRF simulations and several models that are available were not supplied to the writer. At least one uniformity model is being revised and validated at Colorado State University, and should be available in the spring of 1978. Conveyance seepage and field tailwater are most often addressed simply as fractions of diverted or applied water.

Root extraction, transpiration, and evaporation do not appear separately in most modeling efforts. Combined transpiration-evaporation (evapotranspiration) can be determined from climatic conditions or evaluation of the porous media physics. Analyses based on climatic data are very simple and commonly used so the relevant models are seldom presented as such. Investigations using soil physics approaches involve more than one process and are, therefore, described in the subsystem level of modeling.

The segregation of models into process, subsystem, and system levels may reflect more of the writer's bias towards the modeling concept than is justified. However, process level models by themselves have only marginal utility in evaluating IRF systems unless the modeler proposes to fabricate new subsystem or system models. Two important exceptions are to be noted. First, deep percolation represents a major component of return flow.

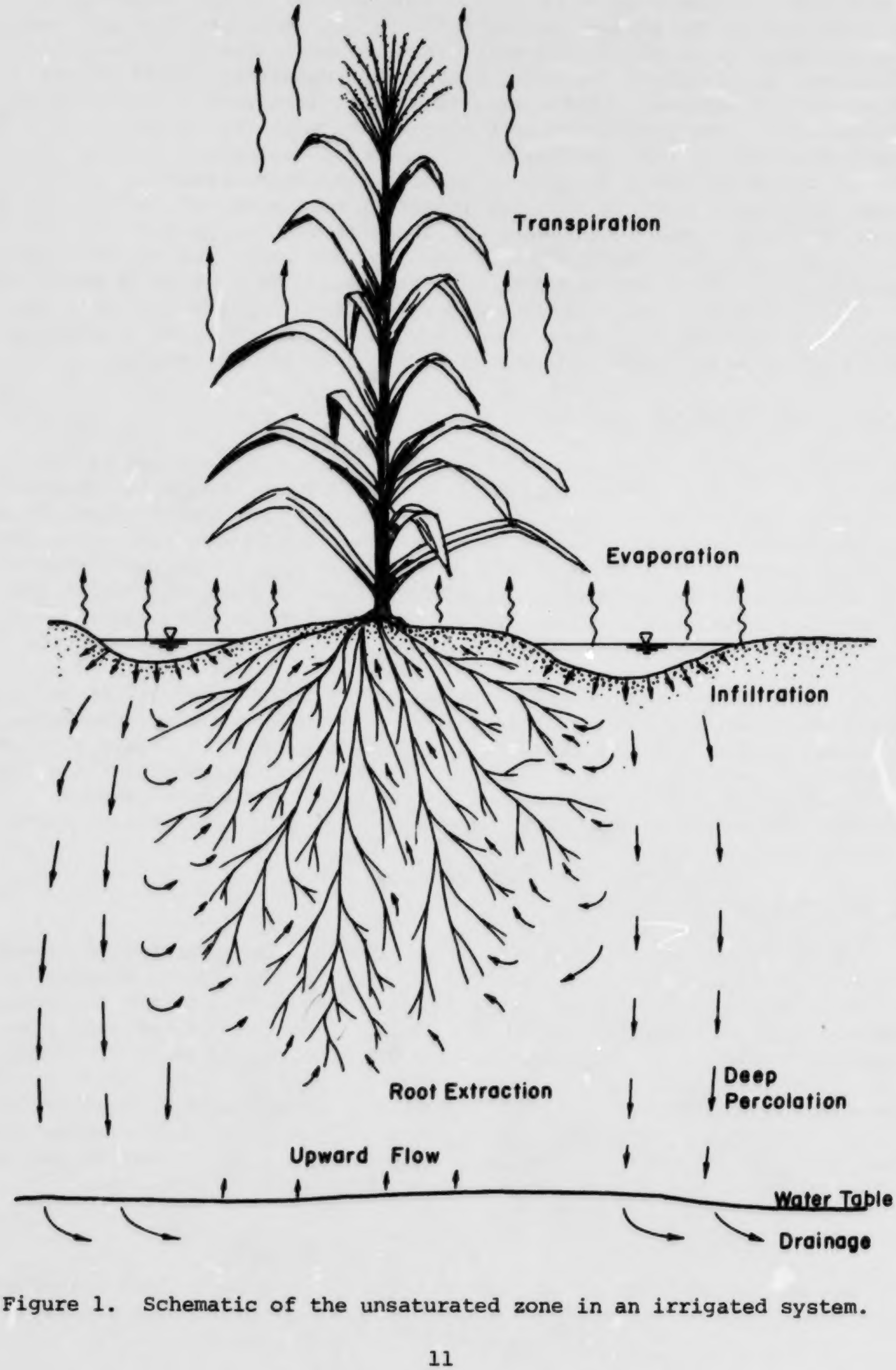
Transpiration
Evaporation
Infiltration
Deep
Percolation
Root Extraction
Upward Flow
Water Table
Drainage

Figure 1. Schematic of the unsaturated zone in an irrigated system.

Analysis of deep percolation or leaching depends on either determining a root zone mass balance or simulating the infiltration-redistribution process. The first alternative requires more data, is more applicable to large scale situations, and is often the most desirable. Evaluating infiltration-redistribution involves shorter time intervals, less data (although more sophisticated), and yields a closer approximation to the actual event. The second exception is the analysis of the chemical-biological aspects of soils and soil solutes. Moisture flow is often better approximated by assuming steady-state conditions or that the transient nature may be represented by a series of steady-state conditions. In these cases, the quality aspects of modeling are somewhat independent of the moisture phase and can be accurately simulated by limiting the scope of the analyses. These types of models are also of benefit when computer time and core capacities are limited. The output of a moisture flux simulation can be input to chemical simulators thereby significantly reducing the dimensionality of the program.

Subsystem Level Models

In this report, the subsystem level of modeling is defined as the combination of two or more process level simulations. The main subsystem for IRF studies is the field hydrology within the irrigated system itself. In a major watershed or river basin, there are other logical subsystems describing precipitation-runoff relations, reservoir operations, in-stream processes like dissolved oxygen behavior, groundwater interflows, etc. Within the irrigation system itself there may be a number of similar subsystems reflecting different soils, crops, and irrigation management practices.

As with any modeling classification, subsystem models vary in the scope and dimension of their mathematics. Some models are detailed treatments of a small part of the irrigated agriculture subsystem shown in Figure 1, others are more macroscopic, large scale and time resolved treatments of the Figure 2 representation. The more detailed models involved basic physics and chemistry whereas the macroscopic approaches are generally mass conservation descriptions.

System Level Models

As the scope and scale of IRF models increase, the variety of models also becomes wider. At the system level, there are two broad classes of models included in this report. The first is the models of the agricultural watershed, shown in Figure 2, in which one or more unsaturated zone subsystems are linked with a groundwater or drainage subsystem simulation to predict total IRF volumes and their time distributions. The second set of system models are those simulating river basin or subbasin hydrologies as shown in Figure 3. In these models, irrigated agriculture represents a small fraction of the actual land area and the emphasis is on evaluating the impact of irrigation on the system rather than quantifying its magnitude.

MODEL EVALUATION

One of the purposes of this project was to make an initial assessment of the various computer programs in order to identify the current modeling

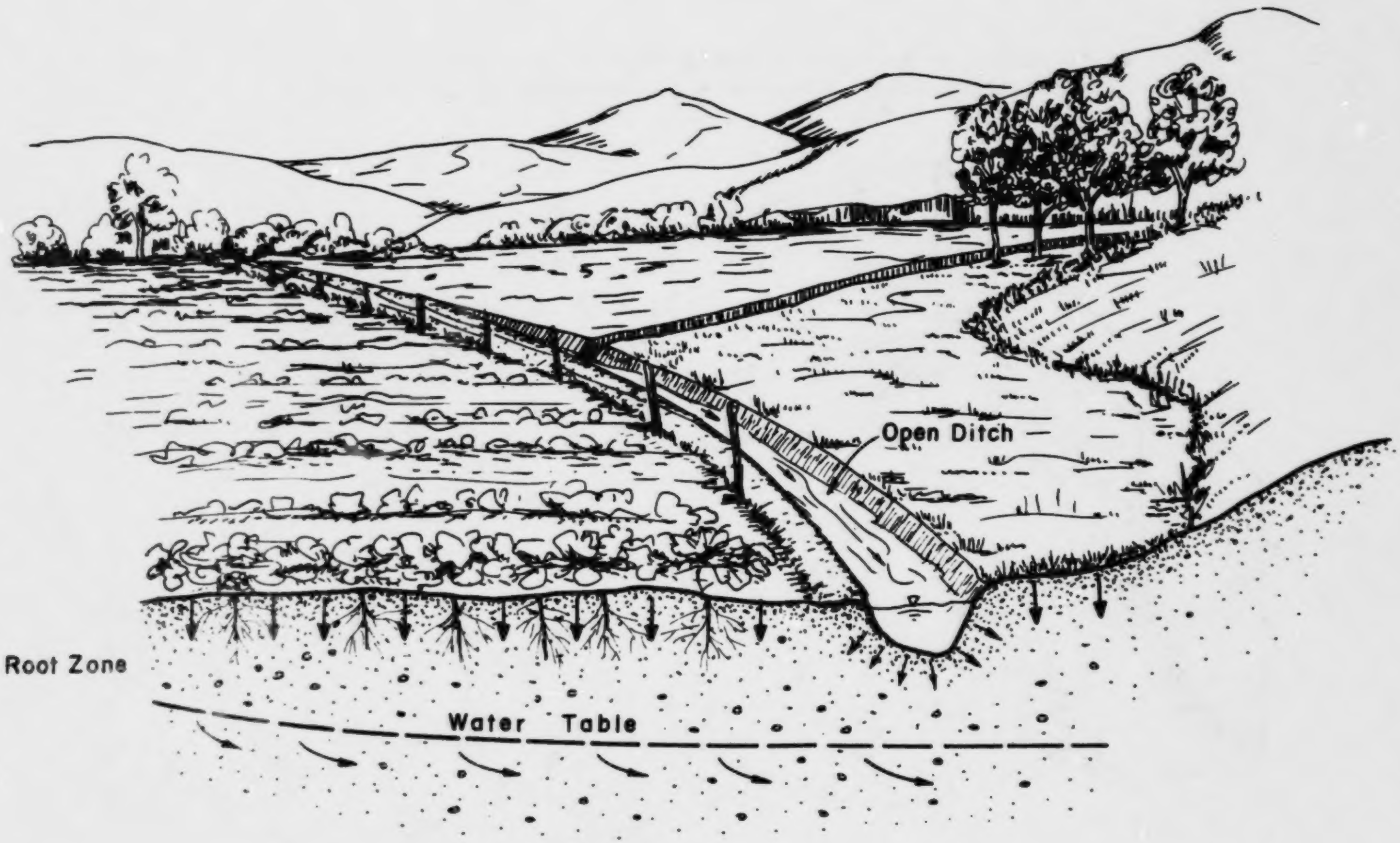
Open Ditch
Root Zone
Water Table

Figure 2. View of a large scale irrigation return flow system.

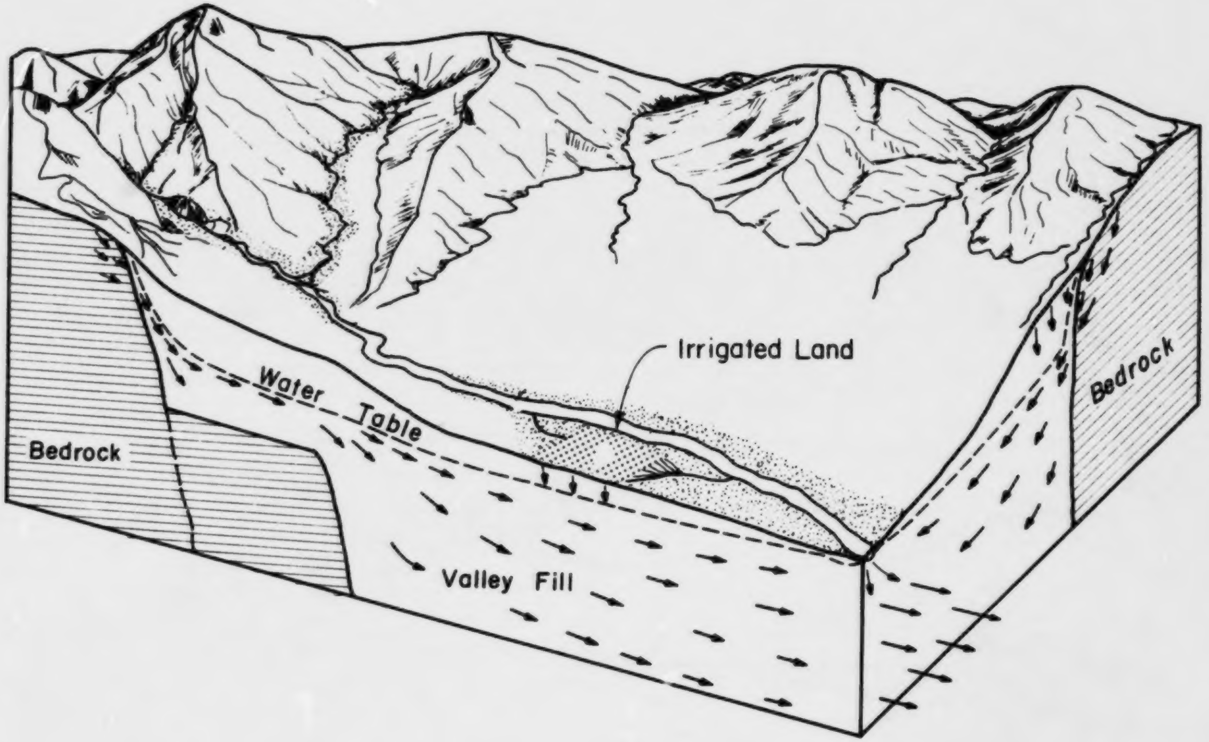
Irrigated Land
Bedrock
Water Table
Bedrock
Valley Fill

Figure 3. An illustration of a watershed which includes an irrigated component (after Eakin et al. (1976)).

capability. Similar studies were examined to determine the alternatives for describing the models. After several revisions, the outline shown in the appendices was selected. The model descriptions are divided into the following eight segments:

(1) Model grouping;
(2) Descriptive or developmental references;
(3) Scope of the model;
(4) Input requirements;
(5) Spatial and time scales;
(6) Structure of the code;
(7) Basic mathematical or analytical approach; and
(8) General comments.

In describing various models, as much as possible of the information presented originates in the cited references in order that descriptive errors are minimized. At the outset, it was desirable to maintain the length of the summaries to one or two pages where possible. This means that the phrases used in describing various aspects of a model must alert the reader's own understanding rather than trying to be exhaustive in detail. Those unfamiliar with a modeling area are encouraged to obtain and review the reference material for a more in-depth assessment. Much of the science behind these models is beyond the training of the writer. As a result, a description's adequacy is highly dependent on the code documentation available with each program. A significant number of the models had little or no documentation which could be used in this report in which case the writer attempted to extrapolate from his own understanding. Under all of these circumstances, it is hoped that the essence of each model has been fairly represented. A summary of the various models' characteristics is given in Table 4.

Model Scope

Under the heading of model scope, a few sentences were developed to describe what the model simulates and its expected output, including the use of input dumps, error flags, and intermediate calculation results to make the model more useable. Most models print input data to insure that it has been input properly. Error flags and results of intermediate computations are not generally included.

Input Requirements

A list of control parameters and basic input data is included to identify to the potential user the information required to utilize the models effectively. This list is not exhaustive, but represents input data of most importance. Occassionally, a series of data is described in more general terms or classified in order to reduce the length of the descriptions.

Spatial and Time Scales

It is important that the "size" of the modeled portion be identified in comparison to the problem's real dimensions. The interval or time scale is also useful in selecting a model to evaluate an IRF problem since detail of

TABLE 4. SUMMARY OF IRF MODEL CHARACTERISTICS

MODEL	FLOWS EVALUATED				STEADY (S) OR TRANSIENT (T)	FORTRAN OR CSMP	RELATIVE SIZE	VERIFICATION REPORTED	DIMENSIONS
	WATER	SALINITY	NITROGEN	PESTICIDES					
A-1	X				T	CSMP	Small	Yes	1
A-2	X				T	Fortran	Medium	Yes	1, 2, 3
A-3	X				T	CSMP	Small	No	1
A-4	X				T	Fortran	Small	Yes	2
A-5	X				T	CSMP	Medium	Yes	1, 2, 3
A-6	X				T	Fortran	Small	No	2
A-7	X				T	Fortran	Small	No	3
A-8	X				T	Fortran	Small	No	2
A-9	X				T	Fortran	Small	No	1
B-1		X			T	Fortran	Medium	No	2
B-2		X			S	Fortran	Small	Yes	1
B-3		X			S	Fortran	Medium	Yes	1
B-4		X			S	Fortran	Medium	Yes	1
B-5			X		T	Fortran	Medium	Yes	1
B-6		X			S	Fortran	Medium	Yes	1
C-1	X				T	Fortran	Medium	Yes	1
C-2	X				T	Fortran	Large	Yes	1
C-3	X (heat)				T	CSMP	Small	No	1
C-4	X				T	CSMP	Small	No	1
C-5	X				T	Fortran	Large	Yes	1
C-6	X				S	Fortran	Large	Yes	1
C-7	X				T	Fortran	Medium	Yes	2
D-1	X		X		T	CSMP	Medium	No	1
D-2	X			X	T	Fortran	Large	Yes	1
D-3	X			X	S	Fortran	Medium	Yes	1
D-4	X		X		T	Fortran	Large	Yes	1
D-5	X (heat)	X			T	CSMP	Medium	No	1
D-6	X			X	T	CSMP	Medium	No	1
D-7	X	X			T	CSMP	Medium	No	1
D-8	X	X			T	CSMP	Medium	No	1
D-9	X		X		T	CSMP	Large	No	1
D-10	X	X			T	CSMP	Small	No	1
D-11	X	X			S	Fortran	Medium	No	2
D-12	X	X			T	Fortran	Medium	Yes	1
D-13	X	X			T	Fortran	Medium	Yes	1
E-1	X				T	CSMP	Medium	No	2
E-2	X				S	Fortran	Medium	No	2
F-1	X	X	X		T	Fortran	Large	Yes	2
F-2	X	X	X		T	Fortran	Large	Yes	2
F-3	X			X	T	Fortran	Large	Yes	2
F-4	X	X			S	Fortran	Large	Yes	2
F-5	X	X			S	Fortran	Large	Yes	2
F-6	X	X			S	Fortran	Medium	Yes	2

the study is directly related to time resolution. The dimension of the simulation may also be provided in this section, thereby indicating the assumptions made about the system's structure.

Computer Code Structure

In these sections, the programming language, core requirements, expected execution times, internal program linkage, and application comments are made. Actually, it was discovered late in the study that core requirements and execution times for the same program will vary substantially from computer to computer. Computer words have different byte lengths and execution times depending on whether or not program compilation is necessary. Consequently, the writer tried to assess these parameters as they would be defined on the CDC 6400 computer at Colorado State University. A major problem occurs when the code is written in a CSMP format because much of the program then becomes part of the basic computer software and storage-time requirements are not known.

Basic Mathematical Approach

It is difficult to express in one or two paragraphs what a complex simulation model accomplished and in what manner. Key phrases and words are used as much as possible to convey to the reader a great deal more than is actually written, and if possible these phrases were taken from the documentation of the code or reference material. The assumptions in a model are at least partially apparent to the already informed reader from the description of what is calculated. Often classical equations in the literature are named without reference. These are noted in the text and generally identify the analytical approach taken.

General

Of general interest to modelers is where the model can be obtained, verification that has occurred, the stage of development and future applications, and special problems that might be encountered in its use. For the most part, this section contains comments on verification and acquisition.

ASSESSMENT OF IRF MODELING

General

If irrigation return flows are to be minimized in an area, the unused diversion should approximate the water necessary to maintain a favorable salt balance in the cropland root zone. The capacity of conveyance and drainage systems should be reduced to the peak seven to ten day average consumptive use rate and the minimal leaching fraction, respectively. Large capital investments in remodeling the irrigation and drainage facilities will have to be made in advance and each irrigator will require substantial retraining. (It can also be successfully argued that the agricultural scientists and engineers would need significantly better practical or "hands-on" training in order to assist the irrigator.) The quality of the flows proceeding to the sequential downstream users will still be somewhat degraded because of the evaporative water depletion, but the effect will be minimized. This objective may appear to be difficult to achieve, however, in at least one instance in western Colorado, there are already authorized plans to invest $100-$200 million into a salinity control project involving 25,000 hectares with the goal that salt loading might be reduced by something on the order of 400,000 metric tons annually. In this particular case and many others of a similar nature, years of investigation preceded the decision for implementation. The dimension of the problem was defined and the effectiveness of the alternative improvements were predicted. The IRF models were instrumental in accomplishing this work and they should continue to be the most important tools available to planners and researchers as they seek to remedy other irrigation return flow problems.

Modeling is the art of model development and testing, but the term "model" itself covers a broad range. In this report, the group of models of interest is the so called "computer models," or those whose mathematical basis is executed by digital computers. These models are developed from concise mathematical expressions of the real system being evaluated, based on the best available evidence of how the system behaves under existing conditions. If the mathematics are correct and general, the same model will predict or simulate the behavior of the real system under changed conditions. Thus, it is possible to expand the information on the system to areas where data have not been collected, thereby yielding a greater understanding of the problems involved in its management.

IRF models can be described in general terms by noting some of the classical methods of model description. None of the models collected for this work or noted in the literature are stochastic in nature. In other words, IRF models are made deterministic by assuming the parameters and variables are uniquely related and are not distributed on the basis of probability. The types of variables and parameters in IRF models are both lumped and distributed depending primarily on the modeler's assumptions regarding homogeneity. Process and many subsystem models have distributed parameter characteristics to separately describe the variation in hydrologic conditions. Some of the subsystem and most of the system level models have lumped parameters because input is usually the average conditions. The solution techniques applied to IRF model mathematics are almost invariably numerical because of the inherent complexity being evaluated. Analytical solutions are possible after comparatively significant simplifying assumptions are made, and these solutions are often utilized to test a more general numerical model. The continuity or time resolution of IRF models also varies with the scale of the simulation. Process models generally approach a continuous simulation by utilizing time increments as small as one-tenth day whereas the system models are generally more discrete as their time increments are on the order of months. Time resolutions are also affected by the dynamic versus steady-state approach being applied. Small time events such as soil moisture flux require a dynamic or time-dependent simulation to evaluate changes. When the only answer sought is the total or aggregate flux from the root zone, a steady-state analysis is often used. Because the steady-state system is generally easier to simulate some models actually "simulate" the dynamic or transient characteristics with a series of steady-state solutions (the CSMP approaches are among the most refined of these approaches).

The IRF system is very complex and not always adequately defined. Studies range in the scope in which the IRF system must be investigated. Consequently, there are numerous models covering the same simulation scope and reflect the understanding and interpretation of the system by the modeler himself. What is not well known at this time is how much difference can be expected when applying these models to the same conditions and which models to apply under various conditions.

Computer Coding

There are basic differences among various modelers in the computer coding approach taken; however, the most significant differences are related to the scope of the model. Process and small subsystem models tend to be straightforward and condition-specific while system level models are usually written to be much more generally applicable. As a result, a great deal more input is required in system level models to define the problem structure and the alternative means for its evaluation.

It appears to be standard practice to utilize subroutines to separate calculations in most FORTRAN models. Data are about equally transferred by the call statement and through common dimensioning. These practices have an advantage that should not be overlooked: the abstraction and individual use of important subroutines by other modelers. Another advantage in actual coding is the relative ease of debugging. A disadvantage is that programs tend to be longer and require more core and time resources.

The use of the IBM simulation language, CSMP, is said to simplify the coding process, but reported comparisons suggest execution times may be greater. The CSMP models cannot be applied to other computers as FORTRAN models can, and this limitation should be strongly considered.

Documentation within the computer code is very useful to users and should be considered. Most IRF models are poorly documented within the code itself.

Probably the biggest problem in the computer codes themselves is that they contain "subtle" programming errors, a misplaced parenthesis, mislabeled statements, redundant looping, etc. This is particularly a problem with large programs. When a model is written and tested, it is unlikely that the modeler's own problem will require looping through each alternative route in the program. The output is corrected for the gross mistakes because they are apparent; the subtle mistakes are much less easily corrected. Thus, when another user applies the model to another set of conditions, difficulty is often encountered. It would be very useful to have several standard data sets on which various computer programs could be tested to evaluate their accuracy, codes, and parameter sensitivities.

The State-of-the-Art

The reader can review the appendix material and several recent reports to decide for himself what the level of technology or state-of-the-art is in IRF modeling. In fact, most reports and papers review the pertinent literature in preparation to presenting their information. Consequently, these next few paragraphs will address the IRF modeling state-of-the-art from a different perspective.

When one contemplates the body of IRF models available today and considers the approach that will be taken in reducing the environmental impact from these flows, it becomes apparent that: (1) the existing models are almost entirely research oriented rather than applied or planning tools; and (2) the most important future need is not in research application but in planning and implementing water quality management strategies. The models require data that are simply not available outside a research investigation and are not easily or inexpensively collected. Areawide planners are not using these models in developing strategies for pollution abatement and risk the possibility that these plans will not be cost-effective. There needs to be an effort made to bridge this gap as soon as possible. The existing models need to be thoroughly evaluated again, their parameter sensitivities quantified, and alternative simplifying assumptions assessed. A new modeling technology designed for planning and large scale evaluation efforts needs to be generated from the research model along with a quantitative description of their functions and expectations. The scientific principles surrounding the IRF system should be reviewed by the consultants and government agencies involved in water quality planning.

Many IRF models demonstrate a noticeable lack of interdisciplinary involvement and yet very good application of interdisciplinary principles. This indicates that literature reviews and professional associations are broad based and active. The use of available computer programs noted by the literature, however, is not generally practiced; rather, most modelers utilize the concepts and mathematics but not the codes themselves. The detailed soil chemistry simulation reported by Dutt, et al. (1972) and Shaffer, et al. (1977) is possibly the best exception. This model has been utilized in studies in several universities and federal research groups. Nevertheless, the central tendency has been to develop individual programs from the common mathematical core. After having reviewed the codes of some 43 of these models, it is the writer's attitude that recoding has been the easiest route because of poor program documentation.

As the reader will become aware in reviewing the appendix model descriptions, there are some modeling phases better developed than others. Estimating the potential and actual evapotranspiration at the soil or crop surface from climatological data is both well developed and tested, but many IRF models employ energy balance or combination equations which require substantially more data than are generally available. The use of the equations relying on available data will not result in significant loss of accuracy if applied properly (although the minimal time increments will be extended). Evaluation of the unsaturated zone hydrology often requires that transpiration and evaporation be separated. Approaches using leaf area index or soil physics have been developed and appear in some of the models included herein. These simulations are more complicated and thus less accurate than climatic functions. The major difficulty lies in root extraction and growth processes. Most models assume uptake is linearly related to the root mass in a soil layer and that the root mass distribution is defined apriori. The more complete models attempt to include submodels of root growth and activity and then introduce stress effects as the limitations of hydraulic conductivity near the roots. In these cases, the summation of uptake is equated to actual transpiration as a check on mass balance and as a means to iteratively distribute the uptake. An interesting sidelight here is the differences in which stress effects are handled in the two approaches. With the climatic estimates, stress is an empirical relationship based on total soil moisture depletion whereas the soil physics approach actually limits transpiration by treating it as a sink term in the moisture flow equation. With adequate data, it should be possible to numerically improve the climatic approach stress function by linking the two methods together.

Within the unsaturated soil profile, infiltration and redistribution of an irrigation or rainfall event occurs over a relatively short period of time (2 to 3 days in many soils). In these situations, evapotranspiration is a small fraction of the moisture movements and is generally neglected. It should be noted that the advent of high frequency irrigation systems remove the acceptability of these assumptions. Nearly every model evaluated in this study encompassing unsaturated flow uses the same form of the one phase moisture flow equation derived by combining the time-depth dependent forms of the Darcy equation and conservation of mass. The soil moisture characteristics (hydraulic conductivity versus soil moisture content versus soil matrix potential) are required for all of these models. These are data universally unavailable outside of study areas. If a rapid in-situ field technique were available, these models would add a great deal to the capability of consultants and planners. The unsaturated soil moisture models solve the nonlinear partial differential equations (for the transient cases) with finite difference, finite element, or the CSMP simulation of sequential steady-state approximations. Numerical dispersion is corrected in a number of ways. Thus, infiltration-redistribution is comparatively well modeled with the most severe limitation being available data.

If the model scope is expanded to where the unsaturated zone subsystem is viewed in the context of its chemical constituent, the reliability is somewhat diminished. The mass transport of the salts, including diffusion and dispersion, is comparatively well simulated by miscible displacement theory. Even the exchange reactions with the soil and solid salt phase, the solution-precipitation of slightly soluble salts, and the formation of ion pairs in the soil solution have been modeled successfully. Some soils contain very large volumes of solid phase gypsum and lime salts adding to the complexity of the salinity modeling, but again verified modeling efforts are reported in the literature. The same is not completely true of solutes involving nitrogen compounds and certain volatile pesticides. Nitrogen transformations are generally simulated with first-order kinetics using rate coefficients reported in the literature or developed in small scale laboratory studies. Denitrification continues to be the most difficult segment of the nitrogen system to model while ammonium and nitrate transport are the easiest. Pesticides often adsorb to the soil matrix and volatilize during their tenure in the soil profile, both processes are evaluated in the existing models.

When the scale of IRF modeling increases beyond the unsaturated zones of the irrigated field hydrology, a great deal of change occurs in the modeling scope. Most of these models are steady-state, lumped parameter types. Their scale represents the simulation of entire fields, valleys, and river basins and the answers sought are those reflecting how irrigation return flows affect the quality of a major flow resource. Input-output or mass balance is the predominant driving force in these system level models. Thus, the detailed simulations at the subsystem and process level are often not directly applicable to large scale models. The problem of how to achieve the proper vertical integration in IRF modeling remains unsolved. There are models of major hydrologic subbasins that include a somewhat detailed subprogram of soil physics and soil chemistry, but add very little, if any, additional modeling capability at this scale because of the difficulty in defining averages on so fine a scale. In a large irrigated region, the "average" is a concept rather than a reality to be used as data for simulating the area. Many IRF models do not encounter this disparity in resolution but it is worthwhile to note nonetheless.

A final point should be made concerning the state-of-the-art in IRF modeling. Verification has been a major effort in the development of process and subsystem models. The system scale models are generally no more than calibrated. The difference being that model output when compared to measured data (verification) is possible when the scope is small, whereas the adjustment of parameters until the predicted output is the same as the measured data (calibration) is the extent of what can be done in simulating large scale systems.

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APPENDIX A

DESCRIPTION OF INFILTRATION-REDISTRIBUTION MODELS

MODEL: A-1

REFERENCES:

Bhuiyan, S. I., E. A. Hiler, C. H. M. Van Bavel, and A. R. Aston. 1971. Dynamic simulation of vertical infiltration into unsaturated soils. Water Resources Institute, Texas A & M University, College Station, Texas. 23 pp.

MODEL SCOPE:

Simulation is of the infiltration into and through a soil profile. Output includes not only the time and spatial distributions of the infiltrated water but the time distributed prediction of the intake relationship.

INPUT REQUIREMENTS:

Input data include moisture content, hydraulic conductivity, and soil suction relations, and initial moisture distribution. Time increments are calculated from user specified error tolerances.

SPATIAL AND TIME SCALES:

Water movement in a one-dimensional unsaturated soil profile is analyzed. Time periods for calculations are in seconds, while output is aggregated up to hours.

COMPUTER CODE STRUCTURE:

CSMP

BASIC MATHEMATICAL APPROACH:

The unsteady infiltration of water into a soil medium is analyzed by assuming a ponded surface, uniform initial soil moisture distribution, and an impermeable layer at the lower soil boundary. The unsaturated soil is then divided into layers for the following two step iterative process. First, the flux between layers is determined using mass conservation, Darcy's Law, and the hydraulic potential between layers. Second, the incremental water content of each layer is then determined by integrating the net flux rate with a fourth order Runge-Kutta method. This updated moisture content is then the initial condition for subsequent iteration.

GENERAL:

The authors note that the program can be modified to handle buried water sources, root extraction, and multi-layered soils. CSMP code is listed in the reference cited above. Verification trials are reported.

MODEL: A-2

REFERENCES:

Brandt, A., E. Bresler, N. Diner, I. Ben-Asher, J. Heller, and D. Goldberg. 1971. Infiltration from a trickle source: I. Mathematical models. Soil Sci. Soc. Amer. Proc., 35:675-682.

Bresler, E., J. Heller, N. Diner, I. Ben-Asher, A. Brandt, and D. Goldberg. 1971. Infiltration from a trickle source: II. Experimental data and theoretical predictions. Soil Sci. Soc. Amer. Proc., 35:683-689.

MODEL SCOPE:

Simulation is of the moisture distribution pattern under a trickle irrigation source. Analysis allows for transient conditions and involves both a plane flow and cylindrical flow description. Hysteresis is neglected. Output includes the time and spatial distribution of soil moisture, evaporation, and deep percolation.

INPUT REQUIREMENTS:

The input data include saturation moisture content, initial distribution of soil moisture, diffusivity and hydraulic conductivity versus moisture content, discharge of the trickle source and its duration and frequency. A number of control parameters set the model in either plane or cylindrical flow coordinates, number of grid points, number and size of time increments, convergence tolerances, number of irrigation cycles, and other geometrical variables.

TIME AND SPATIAL SCALES:

Analysis of the trickle system is based on the application and redistribution of the irrigation water. Calculations are based on small intervals (minutes or seconds) but the basic interval is the irrigation frequency. Model is a two-dimensional treatment of the root zone.

COMPUTER CODE STRUCTURE:

The code is a Fortran IV program using several subroutines with call statement data transfer and several functions using common data linkage. Core requirements and execution time are not discussed.

BASIC MATHEMATICAL APPROACH:

The transient infiltration and redistribution from a trickle irrigation source is simulated with a conventional diffusion type water flow equation using a finite difference technique (a combination of the noniterative alternating directions (ADI) procedure with a Newton-Raphson technique). Boundary conditions describe the trickle emission and evaporation, and the soil conditions surrounding the expected wetting zone.

GENERAL:

The model has been verified against field data and utilized by several other users. The code must be requested from the authors.

MODEL: A-3

REFERENCES:

Hillel, D. 1977. Computer Simulation of Soil-Water Dynamics. International Development Research Centre, Ottawa, Canada. pp. 35-60.

MODEL SCOPE:

Analysis is of the isothermal evaporation from a bare soil water under fluctuating evaporation potential. Soil is homogeneous and isotropic. Output includes the soil surface evaporation and the time-spatial distribution of soil moisture in the soil profile.

INPUT REQUIREMENTS:

The model requires definition of the system geometry (depth of soil profile and number of layers, thickness of layers if not uniform), moisture content, hydraulic conductivity, and moisture suction relations, initial moisture distribution, time distributed evaporation demand at the surface, and the air dry matric potential. If hysteresis is to be considered, additional soil moisture-matric suction tables must be supplied to define the sorption-desorption relationships.

TIME AND SPATIAL SCALES:

The calculations occur on one second intervals with aggregation to days if desired. The spatial scale is a one-dimensional treatment of a 1-2 meter unsaturated soil profile.

COMPUTER CODE STRUCTURE:

CSMP

BASIC MATHEMATICAL APPROACH:

The soil profile is divided into compartments or layers. Movement between compartments follows Darcy's Law and conservation of mass. The computation procedure follows a sequential or iterative evaluation of compartment moisture content and then calculation of flux between compartments based on averaged gradients and hydraulic conductivity. The evaporation rate from the soil surface is set equal to the potential rate when the top layer's soil moisture level is above the air-dry value. If below, the evaporation rate is set equal to the flux into the upper layer.

GENERAL:

The model was numerically tested with and without hysteresis, but no field verification is reported. Results show significant effects and might be usefully applied elsewhere in evaluating hysteresis. The CSMP code is listed in the reference.

MODEL: A-4

REFERENCES:

Lomen, D.O. and A.W. Warrick. 1974. Time-dependent linearized infiltration: II. Line Sources. Soil Sci. Soc. Amer. Proc., 38:568-572.

MODEL SCOPE:

Analysis of infiltration and redistribution of irrigation water from a line source such as multi-outlet trickle irrigation lateral is presented. Moisture flux or matrix flux potential is the primary simulation variable. Flux is expressed in relation to time and distance from the sources.

INPUT REQUIREMENTS:

Input to the model includes the following: (1) number of line sources; (2) line at which computations start; (3) distance between lines; (4) real dimension grid width, depth, and time; and (5) soil hydraulic properties. Some input is required for checking of various numerical functions.

SPATIAL AND TIME SCALES:

Spatial scale varies from the width of an irrigated field to the unsaturated depth. Time scale encompasses the duration of an irrigation.

COMPUTER CODE STRUCTURE:

Written in Fortran IV and using 26 k bytes of storage and approximately 1-2 minutes of central processor time, program is easily adaptable to various computers. A main program coordinates functions through call and common information exchange.

BASIC MATHEMATICAL APPROACH:

The computer code solves the line source infiltration problem on the assumption of step input of irrigation water and a linearized relationship between hydraulic conductivity and moisture content. These assumptions allow analytic solution to the matric flux potential relation as described in the reference cited above.

GENERAL:

Program copy requests should be addressed to the authors cited above. Verification has been made with field data but not reported at the time of this writing.

MODEL: A-5

REFERENCES:

Van Der Ploeg, R. R. and P. Benecke. 1974. Unsteady, unsaturated, n-dimensional moisture flow in soil. Soil Sci. Soc. Amer. Proc., 38:881-885.

MODEL SCOPE:

Simulation is of one, two, or three dimensional unsteady, unsaturated flow in soils. Output includes the time and spatial distribution of moisture contents and fluxes. Four individual models are actually available: (1) 1-dimensional absorption; (2) 3-dimensional absorption (spherical); (3) 2-dimensional infiltration from a line-source; and (4) 3-dimensional infiltration from a point source. The analytical structure is the same in every case so these models will be presented collectively.

INPUT REQUIREMENTS:

The potential user must divide the soil profile into "compartments" with a parameter. The multi-dimensional analysis requires definition in each dimension. The hydraulic properties of the soil such as moisture content dependent conductivity and diffusivity must be defined. Initial conditions through the profiles as well as the distributed input at the surface are also supplied.

SPATIAL AND TIME SCALES:

The analysis is carried out in fractions of an hour with integrated output in intervals of hours or days. Spatial scales are limited to a small region examined in one, two, or three dimensions.

COMPUTER CODE STRUCTURE:

All four codes are written in the IBM 360/365 version of CSMP. Execution time for the simplest model is about 10 minutes.

BASIC MATHEMATICAL APPROACH:

The compartment approach described herein is discussed for other CSMP models included in this work. The profile is divided into segments depending on the dimensionality of the model and defined with respect to their initial hydraulic properties. Then, the ratio of moisture movement between compartments is calculated on the basis of Darcy's Law and conservation of mass by assuming the hydraulic gradient, diffusivity, and hydraulic conductivity are the average between compartments. For small time increments, the moisture content in each compartment as computed by summing the fluxes into and out of the compartment. The procedure is then repeated for each compartment until the desired time of examination is reached. These models utilize a fourth order Runge-Kutta integration method to sum events and do not rely on constant time or step sizes.

GENERAL:

Models have been calibrated and verified against field data in several places. The code listing is contained in the reference.

MODEL: A-6

REFERENCES:

Warrick, A.W., 1974. Time-dependent linearized infiltration. I. Point Sources. Soil Sci. Soc. Amer. Proc., 38:383-386.

MODEL SCOPE:

Simulation is of infiltration and redistribution of irrigation water from a point source such as a trickle irrigation emitter. Input dump and system test are provided. Model will simulate single or multiple outlets.

INPUT REQUIREMENTS:

The program first requires a series of arrays to test the numerical integration and exponential functions. The number of points, strength or discharge, dimensionless depth, radius, and time points are defined. Corresponding to each point defined, the associated initial conditions are read. Use of the program requires that both the hydraulic conductivity and the moisture content versus pressure head relationships be known.

SPATIAL AND TIME SCALES:

The analysis involves the two-dimensional simulation of soil moisture flux into a soil of known properties during a single or multiple irrigation event. The linearized analysis allows multiple points to be evaluated.

COMPUTER CODE STRUCTURE:

The code consists of a main program and functions served by common and call data transfer. Approximately 25 k bytes and 10-20 central processor seconds are required to operate the model.

BASIC MATHEMATICAL APPROACH:

Analytic solutions developed and reported by the author based on the assumptions of step-input of irrigation water and linear relationship between hydraulic conductivity and moisture content. See model A-4.

GENERAL:

This analysis is most applicable where moisture content changes are small such as a high frequency or trickle irrigation systems. Computer code must be requested from the original source. Limited verification has been accomplished.

MODEL: A-7

REFERENCES:

Warrick, A.W., and D.O. Lomen. 1976. Time-dependent linearized infiltration: III. Stip and disc sources. Soil Sci. Soc. Amer. Proc., 40:639-643.

MODEL SCOPE:

Simulation is of disk sources of moisture input at the soil surface. Analysis is three-dimensional. Parameters included in simulation are primarily matric fluxes as a function of depth in soil and distance (radius) from the source origin. Input dump and error flags are incorporated.

INPUT REQUIREMENTS:

The user first specifies the number of values of disc radius to be evaluated, and the number of dimensionless radii, depths, and times. Dimensionless parameters require knowledge of the hydraulic conductivity-pressure head relationship and the hydraulic conductivity-moisture content function. The values of radius, depth and time (dimensionless) representing initial soil moisture conditions are then read in at each grid point established.

SPATIAL AND TIME SCALE:

The model is a three-dimensional simulation of soil moisture flux during an irrigation interval. System solution allows the additive feature so that sequential and parallel disks can be evaluated.

COMPUTER CODE STRUCTURE:

The program incorporates a main program and function routines using common and call data transfer. Code is written in Fortran IV and uses 40 k bytes and 5-10 central processor seconds per analysis. Program is usable in most computer systems as currently written.

BASIC MATHEMATICAL APPROACH:

The generally accepted moisture flow equation for the time-dependent case becomes a linear differential equation if the hydraulic conductivity is assumed linearly related to moisture content. This assumption allows the matric potential to be described by analytic solutions which are discussed in the reference. (See model A-4.)

GENERAL:

Code must be requested from the authors.

MODEL: A-8

REFERENCES:

Warrick, A.W., and D.W. Lomen. 1976. Time-dependent linearized infiltration: III. Strip and disc sources. Soil Sci. Soc. Amer. Proc., 40:639-643.

MODEL SCOPE:

Simulation is of infiltration from a strip source of finite width located on the soil surface. Analysis is two-dimensional. Parameters included in simulation are time distributed soil-water flux and potential.

INPUT REQUIREMENTS:

The user specifies the increments in a trapezoidal integration formula, tolerance for convergence, and strip width as cards in the program. As input, the program needs the number of dimensionless x, y, z, and T values at which solutions are to be determined, the number lines in the analysis, and the values of the dimensionless variables. Each parameter is an array defining values of the parameters at grid points. Each dimensionless parameter is determined from the soil moisture characteristics (hydraulic conductivity, moisture content, and pressure head relationships).

SPATIAL AND TIME SCALES:

Simulation interval is specified by the user although it would be normal to model a single irrigation event. The two-dimensional nature of the model provides a realistic examination of water distributions over an irrigated field.

COMPUTER CODE STRUCTURE:

The computer program utilizes a main program and function routines with both common and call data transfer. Program is written in Fortran IV. Central memory requirements are 24 k bytes and execution time is on the order of 5-10 central processor seconds per analysis. Program is readily adaptable to other computer systems.

BASIC MATHEMATICAL APPROACH:

The generally accepted moisture flow equation for the time dependent case becomes a linear differential equation when it is assumed that the change in moisture content with matric flux potential is linearly related to the changes in hydraulic conductivity and moisture content. This assumption is realistic only when moisture content variations are small such as under high frequency irrigation systems. Applications to the soil system are assumed to be at a steady rate over the interval of simulation.

The solution to the linearized, time-dependent moisture flow equations are analytical and presented in the cited reference. (See model A-4.)

GENERAL:

Computer code must be obtained from the authors.

MODEL: A-9

REFERENCES:

Wind, G. P., and W. Van Doorne. 1975. A numerical model for the simulation of unsaturated vertical flow of moisture in soils. J. of Hydrology, 24:1-20.

MODEL SCOPE:

This model simulates the non-steady unsaturated vertical flow in soils. The model utilizes flow velocity rather than flux to simulate the time and spatial distribution of water in the profile down to a water table. Outputs include the infiltration, vertical movement, water table depths and flux. Soil conditions at each depth increment are also printed. Root extraction and evaporation are not included.

INPUT REQUIREMENTS:

The user must specify the initial soil moisture, groundwater and surface conditions, soil hydraulic properties (conductivity versus moisture tension and moisture content versus moisture tension), irrigation or rainfall characteristics, geometry of the system (layers and time increments), and duration of the simulation. A number of problems can be evaluated during the same run.

TIME AND SPATIAL SCALES:

This model simulates a one-dimensional view of the unsaturated zone. Time increments of fractions of a day are integrated over the irrigation or rainfall interval.

COMPUTER CODE STRUCTURE:

Program is written in FORTRAN for a CDC 6600 computer. Formulas for storage and execution times are given in the reference. Code consists of a main program and subroutine. Data is transferred with common storage blocks. Input is accomplished with cards.

BASIC MATHEMATICAL APPROACH:

The basic mathematical expressions utilized by the model are: (1) Darcy's equation for vertical flow velocity; (2) exponential relationship between hydraulic conductivity and moisture tension; (3) conservation of mass; and (4) Hooghoudt drainage formula. The computation procedure begins with the existing soil moisture distribution and the surface input conditions. The soil is divided into compartments and the moisture contents and hydraulic conductivities for each defined. Based on averages between compartments (to determine gradients) the intercompartmental flux is computed. The compartmental moisture content is then redefined based on net input-output and the procedure is repeated for the next time increment. Deep percolation is the flow passing the last unsaturated boundary. Infiltration is the flow passing the first boundary.

GENERAL:

The computer program is given in the reference cited above. No verifications are actually reported, although sensitivity and accuracy are discussed.

APPENDIX B

DESCRIPTION OF UNSATURATED SOIL SOLUTE CHEMISTRY AND TRANSPORT MODELS

MODEL: B-1

REFERENCES:

Dugard, J. D., and M. Reeves. 1976. Material transport through porous media: a finite-element Galerkin model. Environmental Sciences Division Publication 733, Oak Ridge National Laboratory, Oak Ridge, Tennessee, March. 201 pp.

MODEL SCOPE:

Simulation is of transient flow of a dissolved constituent through either saturated or unsaturated porous media. Transport mechanisms include advective transport and hydrodynamic dispersion. Reactions with the porous media include chemical adsorption and radioactive decay (if applicable). The output describes the time and spatial distribution of the solutes. The moisture flow simulation must be handled with another model. The authors refer to such a model but it is not incorporated in this work.

INPUT REQUIREMENTS:

Data must be supplied to define the geometry and initial conditions of the problem. Also the properties of the media and solute require definition. The soil moisture flux is supplied from the output of another program with tape storage. Some of the important soil properties are tortuosity, bulk density, porosity and dispersion coefficient. The characteristics of the material being transported include its molecular diffusivity parameters, radioactive decay rates as applicable and a distribution coefficient for the linear adsorption function.

TIME AND SPATIAL SCALES:

The problem simulated by this model is two-dimensional and of the size encompased by a field-stream system. Time increments are set in the program for calculation purposes, but the period being simulated can extend from hours to many years.

COMPUTER CODE STRUCTURE:

The program consists of 15 subprograms written in Fortran IV and using common and call data transfer. The code is comparatively large (about 2,000 lines) but does not appear to use more than 100-150 k bytes. Execution times are dependent on the interval being simulated.

BASIC MATHEMATICAL APPROACH:

With the water flow phase being given as input, the equations of flow describe the mass flux of the solute. Flux is divided into diffusive flux and advective flux. Diffusive flux is calculated with a hydrodynamic dispersion tensor and advective flux is equal to the Darcy flux of the water times its concentration. Adsorption is based on a linear function by assuming the ratio of per unit mass of solid adsorption to the concentration is constant. A retardation factor is defined as a linear relationship to the adsorption constant to delay breakthrough of the constituent. Some simplification in the mathematics is achieved by assuming the soil is isotropic with respect to dispersivity.

The integration of the differential equations in the spatial frame is accomplished with the Galerkin finite-element technique using a weighted-residual method. Some of the boundary conditions are of the seepage face and Dirichlet type.

GENERAL:

The program is demonstrated for the case of seepage return flow to a stream. No verification is reported although the numerical solution agreed well with an analytic solution to the problem studied. The program is contained in the reference.

MODEL: B-2

REFERENCES:

Jurinak, J. J., S. Lai, and J. J. Hassett. 1973. Cation transport in soils and factors affecting soil carbonate solubility. EPA-R2-73-235, Office of Research and Monitoring, U.S. Environmental Protection Agency, Washington, D.C. May. 87 pp.

MODEL SCOPE:

Simulation is of cation transport in soils including processes of miscible displacement and cation exchange (both linear and nonlinear exchange isotherms). Output includes the time and depth distribution of solute and exchange cation concentrations and an input dump. Flow is assumed steady. The nonlinear exchange function is a "Kielland" type.

INPUT REQUIREMENTS:

User specifies an alphanumeric identification of the analyses, depth and time increments, total number of time and depth increments, and output frequency control parameters. If the Kielland function is used, the input data set should also include two coefficients for the function. If the linear isotherm is used, two other coefficients are needed (slope and intercept). The model must be supplied with the dispersion coefficient, median flow velocity, bulk density, pore fraction, total cation concentration in solution and the exchange capacity.

TIME AND SPATIAL SCALES:

This model is a one-dimensional analysis of cation transport in soils. The time scale for calculations would be on the order of minutes with output in hours.

COMPUTER CODE STRUCTURE:

Two similar codes are presented in the reference cited above (one for each exchange function). Written for the UNIVAL 1108 computer in Fortran IV, the codes are very small (probably less than 10 k bytes) with execution times ranging from a few seconds to several minutes depending on the time increment control parameters. Programs can be easily adapted.

BASIC MATHEMATICAL APPROACH:

A material balance equation is written in an explicit finite difference form to describe the exchange and miscible displacement of a steady downward flux. Numerical dispersion is eliminated with proper grid spacing.

GENERAL:

The computer programs are contained in the reference. Verification is reported with laboratory data.

MODEL: B-3

REFERENCES:

Oster, J. D., and B. L. McNeal. 1971. Computation of soil solution composition variation with water content for desaturated soils. Soil Sci. Soc. Amer. Proc., 35:436-442.

Oster, J. D., and J. D. Rhoades. 1975. Calculated drainage water composition and salt burden resulting from irrigation with river waters in the western United States. J. Environ. Qual., 4:73-79.

MODEL SCOPE:

This simulation involves the salinity composition of root zone drainage flows. Parameters include dissociated ionic species, gypsum and lime dissolution/precipitation, SAR, CO_2 partial pressure at bottom of root zone (Pco_2), pH, EC, TDS, ionic strength, activities, and activity coefficients. Output also includes $CO_3^=$ and HCO_3^- ion pairing, and 1st and 2nd dissociation constants for carbonic acid. The computer code features an input dump, error flags for iterative sections, but no intermediate results.

INPUT REQUIREMENTS:

Control parameters are provided so a user may include magnesite (not fully developed) and forced saturation of soil lime. Up to 100 individual analyses can be run without dimension and common modification. Data include an identification of the test, Pco_2 at lower root zone boundary, pH, Na^+, Mg^{++}, Ca^{++}, K^+, HCO_3^-, Cl^-, and $SO_4^=$ in applied irrigation water, and the estimated leaching fraction.

SPATIAL AND TIME SCALES:

Simulation is of a single or representative site in an irrigated field. Analysis is steady-state and encompasses the drainage period of the irrigation interval. Model is one dimensional.

COMPUTER CODE STRUCTURE:

Internal program linkage is accomplished by subroutine and functions with common data transfer. The program can be easily adapted, all or in part, to other computer systems or programs. Approximate core and execution time requirements are 70 k bytes and 10-15 central processor seconds, respectively. Programmed originally for an IBM 360 computer using a Fortran IV language.

BASIC MATHEMATICAL APPROACH:

The basic modeling approach along with important assumptions, supportive literature, and data requirements is well described in the previously cited references. The interested user is therefore referred directly to these sources for more detailed information. In general terms, the computations begin by pre-concentrating the ions in the irrigation water by dividing each by the leaching fraction. Then an iterative procedure (governed by convergence tolerances on ionic charge balance, changes in ionic concentrations for Ca and CO_3, and dissociation constants) is used to compute the salinity constituents in the drainage. The extended form of the Debye-Huckel equation is utilized to calculate activity coefficients in the equilibria analyses. Gypsum and lime precipitation/dissolution is used to achieve convergence. Leachate pH is governed by the soil lime equilibria and cation exchange is not included.

GENERAL:

The computer code is available from the authors cited above. Documentation within the code is excellent and substantial verification trials are reported to demonstrate the utility and limitations of the model.

MODEL: B-4

REFERENCES:

Rai, D., and W.T. Franklin, 1973. Program for computing equilibrium solution composition in $CaCO_3$ and $CaSO_4$ systems from irrigation water compositions. Water Management Technical Report No. 29. Colorado State University, Fort Collins, Colorado. October. 42 pp.

MODEL SCOPE:

Simulation is of the salinity composition of root zone drainage. Parameters include dissociated ionic species, gypsum and lime dissolution - precipitation, SAR, pH, EC, TDS, ionic strength, activity, and activity coefficients. Output includes $CO_3^{=}$, HCO_3^{-}, and $SO_4^{=}$ ion pairing with Ca^{++}, Mg^{++}, K^+, and Na^+. The computer code features an input dump, error flags for iterative sections, but no intermediate results.

INPUT REQUIREMENTS:

The program does not include any control options. Input data are sample identification, total concentrations of Ca^{++}, Mg^{++}, Na^+, K^+, HCO_3^-, $SO_4^=$, and Cl^- in the irrigation water, CO_2 partial pressure, and the leaching fraction. Units are in equivalents per liter except for CO_2 (atm) and leaching fraction (expressed as a fraction). Program operates on one sample during each run.

SPATIAL AND TIME SCALES:

The simulation involves a single or average condition in an irrigated field on a one-dimensional basis and steady-state system is assumed.

COMPUTER CODE STRUCTURE:

The code consists of only a main program in the latest version, although the program in reference cited above contained a subroutine for solution of cubic roots. The program can be easily modified for use on computers other than the CDC 6400 at Colorado State University. Core requirements are approximately 30 k bytes. Execution time per run is 15-70 central processor seconds. Code language is Fortran IV.

BASIC MATHEMATICAL APPROACH:

The basic modeling approach, along with pertinent assumptions and simplifications, is well documented in Rai and Franklin (1973). Program is now revised to include nesquehonite. Computations begin by preconcentrating ionic concentrations in the irrigation water by dividing each by the leaching fraction. Ionic strength and activity coefficients are initially calculated by assuming no pairing. Then, a three-dimensional successive approximation loop is entered in which calcium equilibrium is used to arrive at leaching water chemistry. The primary loop flow involves (1) computation of free anions; (2) calculation of free cations; (3) calculation of charged ion pairs; (4) calculation of ionic strength; and (5) calculation of activity coefficients. Then, lime or gypsum equilibrium is checked. If solution is in equilibrium, the program goes to next calcium system or concludes. If nonequilibrium exists, approximations resume at beginning of loop. The Debye-Huckle equation is used for activity coefficients and literature references for equilibria constants are used for the calcium system. Cation exchange is not included.

GENERAL:

The code is available from the authors cited above. Code is moderately documented itself whereas the reference is extensive. Model has been verified against literature and field data. This program is also available for an HP 9825 programmable calculator from the writer.

MODEL: B-5

REFERENCES:

Saxton, K.E., G.E. Schuman, and R.E. Burwell. 1977. Modeling nitrate movement and dissipation in fertilized soils. Soil Sci. Soc. Amer. Proc., 41:265-271.

MODEL SCOPE:

Simulation is of the nitrate-nitrogen-occurrence, movement, and dissipation in 1-2 meters of the unsaturated zone under fertilized agricultural lands. Processes included in the model are solute transport (infiltration, redistribution, and percolation), crop uptake, disposition, of added fertilizer, rainfall additions, mineralization and nitrification. Denitrification, fixation, and runoff losses were assumed negligible. Other nitrogen processes were considered negligible. The moisture flow requirements must be input to the model and must include soil evaporation, plant adsorption from each 15 cm layer, infiltration, soil moisture redistribution between layers, and soil moisture in each layer.

INPUT REQUIREMENTS:

Water flow data for this model comes from the model described by Saxton, et al. (1974). Output from that model or similar daily values for uptake by soil segment, infiltration, soil moisture storage volumes, and deep percolation must be incorporated. Then, the time distributed data describing nitrogen additions to the system, total and depth distributed plant uptake of nitrogen, and the initial nitrogen profile in the soil are read.

TIME AND SPATIAL SCALES:

Daily calculations are made of a one year event in a one-dimensional, transient, unsaturated zone.

COMPUTER CODE STRUCTURE:

Using a main program to read tape output from the soil moisture model, the general nutrient calculations are carried out in subroutines using common and call statement data transfer. Execution times for the Fortran Code are on the order of 10-20 seconds. Core requirements should not exceed 50-60 k bytes.

BASIC MATHEMATICAL APPROACH:

Nitrogen transport is based on the assumption that within each 15 cm soil segment, the concentrations of nitrate are uniformly distributed. Thus, nitrates leaving or entering a layer are calculated as the product of the moisture movement and the existing nitrate concentrations. New concentrations are computed for each hour and soil layer to aggregate the transient system on a daily basis. The withdrawal of nitrates from the soil layers is assumed proportional to water absorption. An annual uptake figure is distributed on a daily basis assuming a proportionality with dry matter production and then distributed in the soil profile according to root distributions. Nitrogen added to the upper soil layers in precipitation or fertilizer moves as indicated above, but ammonium fertilizers are assumed to be either adsorbed or converted to nitrate. A first order temperature dependent decay function was used to describe the ammonium conversion to nitrate. A 10% loss due to volatization was assumed on initial application. Mineralization is fixed at 52 kg/ha per year within the upper soil layer and is distributed with time proportionally to the temperature in the soil between May and September.

The calculation proceeded in the following sequence: fertilizer addition, mineralization addition, uptake, infiltration addition and transport, and transport by redistribution and percolation. A revised nitrate profile is calculated after each process and printed at the day's end.

GENERAL:

The model has been verified (with good agreement) with field data from two watersheds. This is a readily usable model only if the moisture flow is supplied by the earlier model. Thus, modifications should be made to operate this one independently for widespread application. Computer codes must be requested from the authors of the cited references.

MODEL: B-6

REFERENCES:

Tanji, K. K., L. D. Doneen, G. V. Ferry, and R. S. Ayars. 1972. Computer simulation analysis on reclamation of salt-affected soils in San Joaquin Valley, California. Soil Sci. Soc. Amer. Proc. 36:127-133.

MODEL SCOPE:

Simulation is of the interaction of soluble salts (Ca^{++}, Mg^{++}, Na^{+}, K^{+}, $SO_4^{=}$, Cl^{-}, HCO_3^{-}, and NO_3^{-}) and Boron in a soil profile. The model was developed to describe leaching processes so the output includes drainage water quality, soil profile chemistry (changes in soluble, and adsorbed salts). It also predicts the depth of leaching water required to achieve specific values of soluble salts, boron, and exchangeable sodium concentrations in the soil profile. Output includes ionic strengths, activity coefficients, ion pairs, stoichiometric solute concentrations (dissociated and undissociated), total soluble cations, SAR, and ESP.

INPUT REQUIREMENTS:

Input data include leaching water salinity composition, initial soil profile salt distribution, depth distributed exchangeable Ca^{++}, Mg^{++}, Na^{+}. cation exchange constants, gypsum content, adsorbed boron, Langmeier constants, and moisture contents at saturation and field capacity.

TIME AND SPATIAL SCALES:

The principal time frame is the period covered by an application of irrigation water and the subsequent leaching. The model is one-dimensional and encompasses the unsaturated zone of depth specified by the user.

COMPUTER CODE STRUCTURE:

The program is a Fortran code without subroutines or user supplied functions. Core and execution times are not given but appear small (40-60 k bytes, and about 1-2 minutes).

BASIC MATHEMATICAL APPROACH:

The soil profile is divided into layers with moisture movement between layers when field capacity is exceeded. A chromatographic approach to salt transport between layers is assumed. Solute from one layer moves into a lower layer, mixes with the resident solution (at equilibrium) and equilibrates.

The calculation of the equilibrium chemistry for the salts utilize the Guggenheim-Davis equation for activity coefficients and experimental solubility and dissociation coefficients. Boron adsorption-desorption is simulated with a Langmeier isotherm.

GENERAL:

Model was verified with field data and has served as a starting point for several steady-state models developed to predict the chemistry of leaching water. Code must be requested from authors cited above.

APPENDIX C

DESCRIPTION OF UNSATURATED ZONE HYDROLOGY MODELS

MODEL: C-1

REFERENCES:

Feddes, R. A. and H. Zaraday. 1977. Numerical model for transient water flow in nonhomogeneous soil-root systems with groundwater influence. Proceedings of IFIP Working Conference on Modeling and Simulation of Land, Air, and Water Resource Systems, Ghent. September. 18 pp.

MODEL SCOPE:

Simulation is of the unsaturated nonhomogeneous soil system under transient input conditions and root extraction. The uptake of water by the root system is incorporated into the one-dimensional moisture flow equation as a sink term dependent on soil moisture head, effective rooting depth, and potential transpiration. Output includes the time and depth distributed soil moisture conditions, the evapotranspiration, and the interactions with a water table.

INPUT REQUIREMENTS:

The soil is divided into 20 increments and described with the following data: pressure head--hydraulic conductivity--soil moisture content relations; root depth with time; a time distributed root depth correction to account for nonactive roots; pressure head at the wilting point, anaerobiosis point, and at the optimal uptake level; initial soil moisture and water table conditions; and potential transpiration.

TIME AND SPATIAL SCALES:

This model is a one-dimensional analysis of the unsaturated zone. Calculations simulate events over a daily period of as long as desired (one year in reference).

COMPUTER CODE STRUCTURE:

The code is a Fortran IV program consisting of a main program and a plotting subroutine. Neither core nor execution times are given but should not be excessive for most computer systems.

BASIC MATHEMATICAL APPROACH:

The one-dimensional soil moisture flow equation is solved by an implicit finite difference technique. The root extraction sink term is essentially the same as described by Neuman et al. (1975) based on earlier work by R. A. Feddes, although slight modifications are made to the effective root distribution. The effect of the water table is to provide upward moisture movement in response to root extractions and downward movement due to deep percolation.

GENERAL:

This is a simplified version of the model described by Neuman, et al. (1975) and Ostrowski (1976) but verification against field data showed better accuracy. Code must be requested from authors cited in reference.

MODEL: C-2

REFERENCES:

Gupta, S.K., K.K. Tanji, D.R. Nielsen, J.W. Biggar, S.C. Simmons, and J.L. MacIntyre. 1977. Field simulation of soil-water movement with water extractions. Water Science and Engineering Paper 4013. University of California, Davis, California. May. 95 pp.

MODEL SCOPE:

Simulation of "infiltration, vertical seepage, and uptake by plants as related to the hydraulic properties of the soil, soil layering, the root growth characteristics of a given crop in a given soil profile, evapotranspiration rates, and frequency, rate, and amount of irrigation," is presented. Outputs, in addition to an input dump, includes hourly values of moisture content, suction, and flux throughout the profile during an irrigation and daily values during nonirrigation periods. Daily mass balances are also given along with distributed totals for each run describing the irrigation input, evaporation and transpiration, and flux at each node. Data may be supplied by disk or cards.

INPUT REQUIREMENTS:

The program requires a number of control parameters to direct the calculations through the alternatives for various steps. First, boundary conditions when not calculated directly must be specified for field and crop conditions. The problem size and decomposition structure is defined next, i.e., distribution of nodes and material numbers above and below each node. Dates for planting and harvesting are also read in; then a series of flags are specified. Leaf-area-index options include direct input of LAI versus time, or a user specified distribution. Partitioning transpiration and evaporation from inputed values of potential evapotranspiration can be either computed with techniques using LAI related energy balance at the soil surface, or an option supplied by the user. Stress effects on transpiration include options for on-off, logarithmic decrease, linear decrease, a combination on-off and linear or a user supplied function. Soil profiles may be either homogeneous, nonhomogeneous, or layered, each of which requires the hydraulic conductivity-moisture content relationship (expressed as polynomials). Root growth options involving a negative exponential relationship, distributed density functions, or a user supplied system is specified and associated data read into the model. Moisture extracted by the rooting system is evaluated in a sink term added to the moisture flow equation. The form of the sink may be a macroscopic Nimah-Hanks type, related to soil suction, or supplied by the user. Associated data would then be necessary to define the pertinent coefficients. Finally, surface boundary conditions describing static, quasi-dynamic, dynamic, or semi-infinite depth must be known.

TIME AND SPATIAL SCALES:

During an irrigation, time increments may be as small as 0.1 to 1.0 hour with aggregated values presented daily. Spatial resolution is a one-dimensional analysis of the unsaturated region below an irrigated surface.

COMPUTER CODE STRUCTURE:

A main program-subroutine system with common and call information transfer constitutes the essential code structure. Code is written in Fortran IV. Execution time and core requirements are not specified in the reference, but neither are expected to be a problem at most computer facilities.

BASIC MATHEMATICAL APPROACH:

Water entering the soil via irrigation or precipitation either redistributes in the root zone or evaporates from the soil surface. Knowing the potential evapotranspiration rate, surface evaporation is delineated by a leaf-area-index related radiant energy balance computation at the soil surface. The moisture not evaporating from the soil surface moves through the soil profile and/or is extracted by the rooting system.

Soil moisture movement in the root zone is simulated with the single phase, time dependent solution to the Darcy equation. A sink term is added to the basic finite difference solutions to accomplish plant uptake. The model handles the sink term in an interesting way. An iterative solution of the $K-\theta$ system is undertaken until a mass balance between internodal flux and total transpiration is accomplished. A similar mass balance relating the moisture remaining after plant uptake with the distribution of moisture in the profile is utilized to iteratively change time resolutions until both estimates are congruent. Thus, the model automatically insures a mass balance by forcing the detached solutions to the flow equations to be in agreement.

GENERAL:

This model is the first phase of a comprehensive study aimed at simulating nitrogen behavior in soils. Verification has been made against very detailed field data, although only at one location. The code reflects a fair state-of-the-art description of the physical processes in the root zone even though more refined treatments of some segments are possible. However, the sophistication among these segments appears quite homogeneous. Although classified primarily as a research tool, the approach allows application to a number of field situations. Code is available from the authors cited above.

MODEL: C-3

REFERENCES:

Hillel, D. 1977. Computer Simulation of Soil-Water Dynamics. International Development Research Centre, Ottawa, Canada. pp. 61-78.

MODEL SCOPE:

Model simulates non-isothermal evaporation from a soil surface based on an energy balance approach. Moisture transport is simulated as a two phase flow problem and soil heat flux is incorporated. Output includes a time and spatial distribution of soil moisture and heat, surface energy balance, and evaporation.

INPUT REQUIREMENTS:

The code requires a description of initial soil moisture condition, soil properties, and atmospheric inputs. Soil hydraulic properties include the moisture conductivity-suction relationship, soil thermal conductivity (air, water, and solids), volumetric heat capacity (air, water, and solids), albedo, field capacity, porosity, surface roughness, soil temperature-water vapor thermal conductivity function, and the geometry of the system being modeled. Atmospheric variables listed as input are time distributed air temperature, dew point temperature, wind speed, and solar radiation.

TIME AND SPATIAL SCALES:

The basic unit of time is one hour with periods of several days being evaluated. The spatial scale is a one-dimensional evaluation of the first 1-2 meters of the soil profile.

COMPUTER CODE STRUCTURE:

CSMP

BASIC MATHEMATICAL APPROACH:

The surface energy balance includes approximately the same approach described by the Penman equation for evapotranspiration. In this case, the model uses more of the analytical functions and less regression type relationships. Water flow occurs according to Darcy's Law and conservation of mass. Heat flow is described by Fourier's Law written in one-dimension.

The modeling approach involves three steps. First, the hydraulic and thermal gradients and associated conductivities between layers are determined based on initial or existing conditions. Then, the heat, vapor, and water flux is determined by multiplying the gradients and conductivities by the time increment. And finally, the contents of each depth increment or compartment are updated by evaluating the net inflows. The volumetric condition of each soil segment is determined based on average gradients existing between compartments. The iterative solution involves a fourth order Runge-Kutta procedure.

At the soil surface, both water and heat fluxes are calculated. Surface temperature is used to segregate the latent heat flux (evaporation) and the sensible heat (soil warming or cooling of the air). The net energy for evaporation at the soil surface and the net vapor transport through the soil profile are successively evaluated with surface temperature as the dependent variable until convergence is satisfied. Then the surface evaporation and soil heat flux are known for this time interval and the calculation proceeds through the soil profile.

GENERAL:

This model is apparently a second or third generation version developed in recent years by various researchers in conjunction with Dr. Hillel. In this reference, the model is applied to a Gilat fine sandy loam soil in Israel and used to evaluate the effect of albedo variance. These results are simulation runs, not calibration or verification trials. Code is included in reference.

MODEL: C-4

REFERENCES:

Hillel, D. 1977. Computer Simulation of Soil-Water Dynamics, International Development Research Centre, Ottawa, Canada. pp. 79-130.

MODEL SCOPE:

Simulation is of infiltration, redistribution, evaporation, and deep percolation in the unsaturated root zone. Output includes the time and spatial distribution of water in the system. Results can be plotted and input data can also be listed.

INPUT REQUIREMENTS:

The vertical soil profile is divided into a number of compartments or layers of variable thickness. Each layer is assumed to have an initial moisture content, but variable values can be assigned. The various layers can also have different hydraulic conductivities if desired. Other input consists of the moisture content-hydraulic conductivity-suction relationships, and the evaporation-rain or irrigation input frequencies.

SPATIAL AND TIME SCALES:

The spatial scale is the one-dimensional compartmentalization of the unsaturated zone under consideration. The governing equations are solved in intervals of one second with periods of several hours or days considered.

COMPUTER CODE STRUCTURE:

CSMP

BASIC MATHEMATICAL APPROACH:

The basic equations of flow are divided into parts. The flux within the soil profile is calculated by the CSMP system of iteratively calculating moisture content, determining average conductivities and gradients, calculating interlayer flux and recomputing moisture contents based on net inflow-outflow. The intensity of rainfall or irrigation is compared to intake rate of the soil surface to delineate infiltration and surface storage. Evaporation at the soil surface occurs at the potential rate (input data) until the upward flux or input is less than this rate. And finally, the deep percolation is taken as the lowest compartment's hydraulic conductivity. Uptake and transpiration are not included. A mass balance is maintained as a check on the computations and output summary.

GENERAL:

Analysis of the model does not indicate either verification or calibration trials. Rather, evaluation of soil types and initial conditions are presented. Code is included in the reference.

MODEL: C-5

REFERENCES:

Saxton, K. E., H. P. Johnson, and R. H. Shaw. 1974. Modeling evapotranspiration and soil moisture. Trans. ASAE, 17:673-677.

MODEL SCOPE:

The simulation is of the evapotranspiration and soil moisture profiles in an irrigated system. Evapotranspiration is determined as the sum of canopy evaporation, soil evaporation, and plant transpiration. Soil moisture is redistributed by hydraulic conductivity-tension functions.

INPUT REQUIREMENTS:

The first input data are the time and depth distributed root distribution percentages to proportion the root water extraction patterns. Then, daily values of potential evapotranspiration are read in based on a suitable approach (combination equation and pan evaporation in this work) as are net radiation values. Then, the data describing the stress curves are read in to adjust the crop transpiration. For each soil type present, the user must detail the conductivity-tension relationship, wilting point, field capacity, saturation and initial soil moisture. Water inputs to the system through infiltration are input along with canopy development curve data. Output can be directed to paper, tape, or both types of printout.

SPATIAL AND TIME SCALES:

The time interval for calculation is one or two irrigation seasons evaluated a day at a time. Spatial scale is a one-dimensional profile through the 1 to 1.5 meter root zone.

COMPUTER CODE STRUCTURE:

The program is contained primarily in a main program of sequential calculations. A series of subroutines using call statement data transfer exclusively perform interpolation and data adjustment functions. Code is written in Fortran IV. Core requirements noted in printout appear to exceed 150 k bytes, but should not exceed 40-50 k in most computers. Execution times are on the order of 10-20 central processor seconds.

BASIC MATHEMATICAL APPROACH:

The basic model calculations involve three sequential steps performed repeatedly on a daily interval: (1) computation of actual evapotranspiration; (2) adding infiltration to soil moisture; and (3) redistributing the soil moisture. Beginning first with input values of potential evapotranspiration, the initial calculations segregate canopy evaporation from soil evaporation and plant transpiration. Maximum interception canopy evaporation is set at 2.5 mm. Potential values for soil evaporation (assumed to come only from first 15 cm) and transpiration are divided according to the canopy shading percentage. Reduction in potential soil evaporation to an actual value is made with a literature ratio expressed as a function of soil moisture. Transpiration is adjusted by crop curves. The daily transpiration (and evaporation in the first 15 cm) is assigned to respective soil segments based on root distributions. These values are then adjusted further for stress using literature relationships. After the root extraction has been deducted from the soil moisture, infiltration due to daily precipitation (or irrigation if present) is evaluated. All infiltration up to 90% of the available capacity in each soil segment is initially stored therein beginning with the top layer. And finally, a four hour steady-state analysis of the one-dimensional Darcy equation for unsaturated flow utilizing the conductivity-tension relationship is used to redistribute the moisture in the profile for the next day's analysis.

GENERAL:

Three years of detailed field data were used to verify the modeling approach. Calibrations showed good agreement with measured data. This model does not include extensive treatment of each individual process which would make it exclusively a research model. The code is available from the authors cited.

MODEL: C-6

REFERENCES:

Trava, T. L. 1975. Allocating available irrigation water on the farm. Unpublished Ph.D. Thesis, Department of Agricultural Engineering, Colorado State University, Fort Collins, Colorado. December. 107 pp.

Jensen, M.E., C.E. Franzoy, and D.C.N. Robb. 1970. Scheduling irrigations using climate-crop-soil data. J. Irr. and Drain. Div., ASCE, 96:25-38.

Kincaid, D.C. and D.F. Heerman, 1974. Scheduling irrigations using a programmable calculator. ARS-NC-12. Agricultural Research Service, U.S. Department of Agriculture. February. 55 pp.

MODEL SCOPE:

Simulation of irrigated crop evapotranspiration is based on climatic data utilized in a combination energy flux-advection model (Modified Penman Equation). Parameters in the analysis include the potential evapotranspiration for 10 field crops, actual use based on stress and growth stage adjustments, predicted dates of future irrigation, and soil moisture status estimates.

INPUT REQUIREMENTS:

The program is set up to compute multiple crop, multiple farm, multiple region irrigation updates and schedules. After this problem structure is defined, the user supplies a region by region function for the average expected evapotranspiration. Then soil moisture, consumptive use, climatic, and irrigation data for the three previous days are read in and evaluated. Crop data are also read in with each run.

SPATIAL AND TIME SCALE:

Evapotranspiration and irrigation scheduling is an areal average, nonspatial computation. Time scale is on a daily basis, and the model is one-dimensional.

COMPUTER CODE STRUCTURE:

Main program and subroutine structure, written in Fortran IV, compromise the Trava version of the model. Common data transfer is primarily employed. Core requirements amount to about 100 k bytes but some of this involves the optimization package incorporated in the Trava model. Execution time is on the order of 50 central processor seconds.

BASIC MATHEMATICAL APPROACH:

During the course of a scheduling run, detailed soil, crop, and climatic data for the period since the last update are used to update the present time frame. The modified Penman Equation is used as the basic tool with stress, recent irrigation, and crop corrections used as described by Jensen, et al.

(1970) and Kincaid and Heerman (1974). The future prediction utilizes the same approach with the exception that a mean expected evapotranspiration function is used instead of the Penman equation.

GENERAL:

The Penman equation is used extensively in the more detailed simulation models and this model's approach to calculating consumptive use is among the most correct. Thus, although it is more of an operational tool, it is included in this writing because of its widespread applicability and basis for consumptive use calculations in other models. Code is only available from the writer.

MODEL: C-7

REFERENCES:

Neuman, S. P., R. A. Feddes, and E. Bresler. 1975. Finite element analysis of two-dimensional flow in soils considering water uptake by roots: I. Theory, II. Field Applications, Soil Sci. Soc. Amer. Proc., 39:224-237.

Ostrowski, J. T. 1976. Behavior of groundwater subject to irrigation of effluent--a case study. M.S. Thesis, Civil Engineering Department, University of Maryland, College Park, Maryland. 121 pp.

MODEL SCOPE:

Simulation is of infiltration, evapotranspiration, root extraction, and soil moisture distribution in an irrigated field. Soil profiles extend to a water table lower boundary.

INPUT REQUIREMENTS:

The geometry of the soil system is first defined by locating a finite element grid. Then the soil hydraulic properties are incorporated (porosities, permeabilities, tension versus moisture content relations, and relative permeability versus moisture content relations). Initial and boundary conditions at each element node require description of potential evaporation and transpiration, infiltration, and flux. And finally, the time limits of each problem are set.

TIME AND SPATIAL SCALES:

The model is a two-dimensional analysis of an irrigated field condition. Calculations are made for a period of hours or parts of hours and extend as long as desired.

COMPUTER CODE STRUCTURE:

The code as modified by Ostrowski (1976) is written in Fortran IV. A main program with subroutines (common and call data transfer) form the basic structure. Execution times are very large, one week, for example, requires 20 mintues. Core requirements are not noted because of tape storage for data, however, the program should be useable on computers with available core in excess of 50 k bytes.

BASIC MATHEMATICAL APPROACH:

The basic soil moisture flow equations are solved using the Galerkin finite element method, using a discretization scheme. Two aspects of the flow equations merit attention here. Potential evapotranspiration in the Ostrowski (1976) version is based on pan evaporation adjusted by a temperature dependent growth index and the porosity-tension characteristics of the soil. Surface evaporation is a prescribed fraction of the total evapotranspiration with potential transpiration being the difference. The uptake of moisture in a soil segment is assumed to be a function of hydraulic conductivity multiplied by the difference in pressure head difference between the root-soil interface and the surrounding soil and divided by a proportionality coefficient describing the exponentially distributed root mass. Actual transpiration is calculated as the maximum sum of water extractions in each soil segment subject to a limit imposed by the potential rate. Evaporation is only allowed to occur in the first soil segment. The flux of water at the soil surface (after evaporation) is an input variable.

GENERAL:

The model in its various forms has been verified against field data at several locations. The practical use of the program, however, is limited by available computer time and the complexity of required data. The code is available from the authors cited above.

APPENDIX D

DESCRIPTION OF UNSATURATED ZONE HYDRO-QUALITY MODELS

MODEL: D-1

REFERENCES:

Beek, J. and M. J. Frissel. 1973. Simulation of nitrogen behavior in soils. Centre for Agricultural Publishing and Documentation, Wageningen, The Netherlands. 67 pp.

MODEL SCOPE:

Simulation is of the nitrogen transformation and transport in cultivated soils under aerobic conditions and having a large buffer capacity. Transport and temperature are modeled with the models described by DeWit and Van Keulen (1975). The analysis involves the microbial decomposition of organic matter, and subsequent processes of mineralization, immobilization, humus formation, nitrification and leaching. Denitrification and the soil pH reactions are not included. Output includes the time and depth distribution of the nitrogen compounds and the removal of nitrogen from the system through leaching. The soil profile is divided into 20 compartments or layers. Nitrogen transformations occur in only the first 4 layers, leaching in all 20, and heat flow in the first ten. Initial conditions limit water content, temperature, and solute characteristics to the same in each layer.

INPUT REQUIREMENTS:

The input data to this model are as follows: layer thickness, initial moisture content, initial nitrate-nitrogen content, initial temperature, heat capacity (water and minerals), relative amount of minerals, initial mass of proteins, sugars, lignin, cellulose and biomass, initial ammonium, number of ammonium oxidizers per soil volume, maximum nitrification rates, bulk density, hydraulic conductivity and diffusivity as a function of moisture content, saturation values, water content at lower boundary, irrigation frequency, irrigation depths, application rates, beginning of irrigation, irrigation durations, maximum hydraulic head at surface, heat conductivities versus moisture contents, time distributions of surface temperature, dispersion and diffusion coefficients, tortuosity, carbon dioxide parameters, and the array of nitrogen transformation coefficients, and decomposition rates.

SPATIAL AND TIME SCALES:

The basic time increment is the irrigation interval evaluated by calculation intervals down to minutes. The simulation is a one-dimensional treatment of the first 1-2 meter crop root zone area.

COMPUTER CODE STRUCTURE:

CSMP

BASIC MATHEMATICAL APPROACH:

Since the water, heat, and mass transport processes are described in this work under the DeWit and Van Keulen (1975) model, this discussion will be limited to the nitrogen system.

Organic matter is assumed to consist of protein, sugar, cellulose, and lignin which resist microbial attack in descending order. Decomposition rates are not dependent on concentrations but are both temperature and moisture dependent. Humus and biomass also represent organic matter; humus the nondecomposable form. The decomposition is a first-order kinetic approach proportional to the amounts of each segment of organic matter available. Temperature and moisture contents other than optimal values are adjusted by proportionality constants. The use of ammonium and nitrate by the biomass is based on carbon/nitrogen ratios and are related by a first-order function of the decomposition rates.

The nitrification segment of the model assumes that nitrate moves with the moisture but ammonium is adsorbed completely (NH_4^+ exchange processes are considered). The rate of NH_4^+ to NO_3^- conversion is determined as the ammonium to nitrate ratio with other reactions occurring faster and, therefore, are ignored. This rate is proportional to the number of ammonium oxidizers and is independent of the ammonium present. Both suboptimal temperatures and moisture content are handled as in the previous paragraph.

GENERAL:

Verification is not discussed. A computer code listing is contained in the reference.

MODEL: D-2

REFERENCES:

Davidson, J.M., G.A. Brusewitz, D.R. Baker, and A.L. Wood. 1975. Use of soil parameters for describing pesticide movement through soil. EPA-660/2-75-009. National Environmental Research Center, Corvallis, Oregon. May. 162 pp.

MODEL SCOPE:

This model simulates the simultaneous transport of water and solutes through a field soil. The analysis describes the transient and interactive nature of the solute-soil matrix system. Assuming isothermal conditions, the simulation evaluates pesticide concentrations in both the solute and soil matrix with time and depth. The transport analysis is a miscible displacement approach including convection, diffusion, mechanical dispersion, and adsorption-desorption. Output from the program includes a partial listing of input control parameters and data, sorbed and solute concentrations as functions of time and soil depth, and intermediate values of coefficients and water-solute flux. Controls are included for iterative calculations.

INPUT REQUIREMENTS:

In addition to a number of control parameters setting up the alternative program options, the user must supply a comprehensive list of soil hydraulic properties, boundary conditions and chemical concentrations and characteristics. A series of optional data sets are necessary depending on the structure of the program selected.

Soil physical and hydraulic data needed include: soil depth, saturated hydraulic conductivity and moisture content, soil evaporation rates and duration, moisture content versus pressure head relationships, moisture content versus hydraulic conductivity data, and bulk density. Boundary conditions include time and depth increments, time and depth limits, initial soil moisture conditions, and characteristics of water applications at the surface. Other input parameters are included in the description of the boundary conditions which establish certain system reactions, but the reader is referred to the reference material for more specific details. The chemical data which are needed in the program consist of dispersion, adsorption, desorption and vapor diffusion coefficients, concentration of pesticide or chloride in the infiltrating moisture, and initial conditions within the soil profile.

SPATIAL AND TIME SCALES:

This simulation is a one-dimensional analysis of pesticide transport through an unsaturated soil profile encompassing a crop root zone and the strata below. Time intervals for intermediate calculations are set by program user but overall simulation encompasses the application-drainage periods.

COMPUTER CODE STRUCTURE:

A main program-subroutine format is used with call and common data transfer. Code is written in Fortran IV. Listing is well documented with comment cards for easy application of the program. Input and output require no special tape or disk apparatus. Model should be easily adapted to computer systems other than the IBM 360 originally used.

Core and execution times are not noted in reference material but do not appear to be limitations for facilities having in excess of 100 k internal memory and allowing several minutes in central processor execution time.

BASIC MATHEMATICAL APPROACH:

The analysis begins by using a Crank-Nicolson implicit finite difference scheme to compute the change in water content as a function of time throughout the soil profile. The moisture flow equation, based on single phase flow and derived from Darcy's equation and mass balance, is evaluated in the soil matrix by solving its analog form (pressure head) and then calculating moisture content using head-moisture content relationships.

The chemical aspects of the problem begin with assumptions that the adsorption-desorption process can be adequately simulated by single-valued functions. Linear relationships are assumed between adsorbed and solute pesticide concentrations when a pesticide-soil characteristic, N, equals 1 (Freundlich Equation). The rate of mass transfer to the adsorbed phase is determined with rate coefficients based on the Arrhenius Equation.

The transport of pesticides in the soil system under transient conditions is described by a miscible displacement equation which includes expressions for convection, diffusion, mechanical dispersion, and adsorption-desorption. The resulting differential equation is solved with an explicit finite difference procedure with a number of steps taken to correct any numerical dispersion that may occur.

GENERAL:

This model has been tested under both laboratory and field conditions. The results appear sufficient to suggest use of the model. The code itself is contained along with its documentation in the reference cited above.

MODEL: D-3

REFERENCES:

Davidson, J.M., G.A. Brusewitz, D.R. Baker, and A.L. Wood. 1975. Use of soil parameters for describing pesticide movement through soils. EPA-660/2-75-009. National Environmental Research Center, Corvallis, Oregon. May. 162 pp.

MODEL SCOPE:

Steady-state soil water condition simulation of pesticide movement through soil. Isothermal conditions are assumed. Simulation includes pesticide concentrations with depth for soil solute and soil systems. Transport analysis includes convection, diffusion, mechanical dispersion and adsorption-desorption. Output primarily consists of solute and sorbed pesticide concentrations with time and soil depth. A simple input dump is included.

INPUT REQUIREMENTS:

Control parameters provide the user with flexibility in describing the initial state of the system. For each run to be made, the user must specify whether solute concentrations versus soil depth or time are to be output. If output is based on time, the number of time increments must also be specified. Then a parameter is used to either generate a chemical concentration at the soil surface or describe an initially distributed concentration. And finally, an initial distribution of relative solute concentration can be read in or the program can put a square pulse distribution in initially. Relative solute concentration is the ratio of actual solute concentration to initial input concentration.

After input of the control parameters, values for flow velocity, dispersion coefficient, adsorption coefficient, water content, bulk density, initial concentration of pesticide, maximum soil depth considered, time of soil application of pesticide, exponents in adsorption-desorption equations, length of initial pesticide distribution, time increment in calculations, and depth increment are entered.

Other optional input data and specific details regarding format and order are given in the previously noted reference.

SPATIAL AND TIME SCALES:

This simulation is a one-dimensional analysis of pesticide transport into and through a soil profile on the scale of crop root zone and the unsaturated regions below. Time scales may be set by user, but in general, the simulation is of the water application-drainage interval. In irrigated systems, the total time scale would approximate the irrigation interval with user supplied increments within this time frame.

COMPUTER CODE STRUCTURE:

Program consists of a main program which coordinates data input and output, sets time and space increments, and makes summary calculations. Two subroutines are included which calculate solute concentrations. Interprogram data transfer is accomplished with call and common statements. Program is written in Fortran IV and is well documented with comment statements. Core and execution time requirements are not given, but appear to be in the range of 50-70 k bytes and 5-15 CP seconds per analysis, respectively. Program does not require tape or disk input-output devices and should be easily adapted to computer systems other than the IBM 360 initially utilized.

BASIC MATHEMATICAL APPROACH:

This analysis assumes a steady-state volumetric soil-water flux as determined by the Darcy Equation. Flow velocity is determined by dividing the flux by the volumetric soil-water fraction. Pesticides enter the problem either as concentrations in applied water or as initial concentrations distributed through the soil profile and transported through miscible displacement. The simulation of adsorption-desorption assumes the process can be represented by a single-valued function for adsorption and desorption and that a linear relationship exists between the adsorbed and solute pesticide concentrations (Freundlich equation).

The transport of pesticide in the soil system occurs through convection, diffusion, mechanical dispersion, and adsorption-desorption. The transient miscible displacement is simplified by assuming that the dispersion coefficient is independent of depth and that the Freundlich adsorption model is adequate. The resulting differential equation is solved by an explicit finite difference procedure which is corrected for numerical dispersion. Specific details of the correction procedure are found in the reference.

GENERAL:

This model along with descriptive material is given in the previously referenced report. Both laboratory and field data were collected to calibrate and verify this model.

MODEL: D-4

REFERENCES:

Davidson, J.M., D.A. Graetz, P.S.C. Rao, and H.M. Selim, 1977. Simulation of nitrogen movement, transformations, and uptake in the plant root zone. Draft Report to the Environmental Protection Agency, Office of Research and Development, Athens, Georgia. 139 pp.

MODEL SCOPE:

Simulation is of the nitrogen cycle in a crop root zone using finite difference approximations to the flow of moisture and convective dispersion and transport of NO_3^- and NH_4^+. Plant uptake and microbiological transformations as well as NH_4^+ adsorption-desorption are also included. Microbial transformations simulated are first-order kinetic approximations of nitrification, denitrification, mineralization and immobilization.

INPUT REQUIREMENTS:

The user must first supply a number of control parameters to set the number of points in the moisture content versus head relationship, initial depth and time increments, plotter control, and the number of points various initial conditions are specified. Then the soil-water hydraulic conditions are input along with initial soil nitrogen conditions, nitrogen transformation rate coefficients (nitrification, immobilization, mineralization, denitrification). The Freundlich distribution coefficient along with various soil properties such as bulk density and depth are also read in as input. The final set of data is the description of the irrigation or rainfall event. These parameters include duration of event, chemistry of applied water, and evaporation.

SPATIAL AND TIME SCALES:

This program simulates the fate of various nitrogen species in the unsaturated crop root zone in a one-dimensional fashion. Each model run simulates an irrigation or rainfall event although a series can be set up to model a longer period.

COMPUTER CODE STRUCTURE:

The computer program consists of a main program with an input section and seventeen subroutines and functions supplied data with call and common statements. Core and execution time requirements are not given but are not expected to restrain use on most computer systems. The program is written in Fortran IV and should be widely adaptable.

BASIC MATHEMATICAL APPROACH:

The moisture flow system is simulated by solving the nonlinear partial differential equation governing one-dimensional unsaturated flow by an explicit-implicit finite difference approximation. The nitrogen transformations involve: (1) nitrification of NH_4^+ to NO_3^-; (2) mineralization of organic N to NH_4^+; (3) immobilization of both NH_4^+ and NO_3^- to organic N, and (4) denitrification of NO_3^- to the gaseous form. Each of these transformations was assumed to be of the first-order kinetic type which assumes optimal pH and temperature conditions. Ammonium ion exchange was considered to be an instantaneous reaction described by a linear Freundlich adsorption relationship. The nitrogen transformation and transport equations are also nonlinear partial differential equations solved by finite difference approximations.

A nitrogen plant uptake phase was also included in the model. The Penman analysis of potential evapotranspiration was used in connection with a Molz-Remson extraction pattern model to determine the ratio and distribution of uptake. A sink term approach was used in the uptake model and it was assumed that root capacity for adsorption was uniform over the length of the system.

GENERAL:

The computer code is published in the reference cited above but is not documented within the code itself. Calibration and verification results are reported.

MODEL: D-5

REFERENCES:

DeWit, C. T. and H. Van Keulen. 1975. Simulation of transport processes in soils. Centre for Agricultural Publishing and Documentation. Wageningen, The Netherlands. 100 pp.

MODEL SCOPE:

The movement of heat, salts and ions, and water in unsaturated soil is described by a series of CSMP coded computer routines. Transport of these materials and energy encompasses diffusion, dispersion, and mass flow. The soil profile is divided into a series of compartments in which a sequential materials balance is computed. A number of the processes are not mutually exclusive, and the writers do not attempt to present a clear description for integrating the system together. Output includes the time and spatial distribution of the parameters. Plotting functions are also described.

INPUT REQUIREMENTS:

1. Soil heat flow: surface temperature fluctuations with time, thickness and number of soil depth increments, thermal conductivity of the soil compartments, and volumetric heat capacities; 2. Salt transport: initial moisture contents, labyrinth factors, initial solute concentrations, inflow volume and concentration, compartment thicknesses, a dispersion factor, and water diffusion coefficients; 3. Ionic diffusion: compartment thickness, diffusion distance, total depth, water contents, labyrinth factor, valency and initial concentrations of the ion under study, and diffusion coefficients; 4. Ionic transport: initial moisture contents, labyrinth factor, compartment geometry, dispersion factor, exchange capacities, water inflow, diffusion coefficients, solution-adsorption site equilibrium constant, and initial distribution of ions in the soil profile; 5. Infiltration: initial moisture contents, compartment geometries, initial water content at the soil surface, hydraulic conductivity and diffusivity functions of water contents.

SPATIAL AND TIME SCALES:

Calculation proceeds in time increments on the order of five to ten minutes and continues through periods of days. The analysis is limited to the 1-3 meter unsaturated zone and is one-dimensional.

COMPUTER CODE STRUCTURE:

Code is written in CSMP with Fortran output. Program is dispersed in the reference and not presented in a single listing. In addition, the five segments noted are not described as an integrated model, although, as will be pointed out next, the basic model structure is the same for each segment. Neither core nor execution times are available.

BASIC MATHEMATICAL APPROACH:

The soil depth is divided into a number of layers or compartments. With this geometry established and the initial conditions defined, the approach is to compute the movements from one compartment to the next based on the gradient between layers, and diffusion and dispersion functions.

In the heat flow submodel, the heat flow rate equals the temperature gradient between compartments multiplied by the thermal conductivity of the soil. The heat energy in a layer equals the temperature multiplied by the volumetric heat capacity multiplied by the compartment size. In order to calculate the heat flow with time, a time distributed surface temperature is defined along with the initial thermal characteristics of each compartment. The dynamic nature of the system does not allow for a direct equilibrium solution describing the heat status at each level in the soil. The procedure utilized is a centralized, forward integration procedure (explicit). At any instant in time the heat contents of all compartments are initially given. From this information the flow rates into and out of each compartment are computed and the volumetric heat contents are iteratively reviewed. The analysis can be for layered soils if their thermal coefficients can be defined.

The salt transport submodel operates in the same manner as the heat flow submodel except that flow is input at the surface (rate) with salt movement between compartments based on concentration differences (diffusion) and mass transport with the flow. Mass balance between compartments is maintained by recomputing salt accumulations. Dispersion due to tortuosity is also related with a coefficient to the concentration gradients.

Ionic diffusion in the absence of moisture flow is also based on the preceding approach with gradients based on ionic concentrations. The ionic transport submodel includes not only ionic diffusion, dispersion, and mass flow but cation exchange as well. Again, the ionic composition of each compartment is iteratively determined in conjunction with the net inflow or outflow as was described for the heat flow submodel. The added complexity of the monovalent-divalent ionic adsorption processes is handled by relating the adsorbed ions proportionally to the moisture content and exchange capacity and then distributing the relative composition of the adsorbed ion in an equilibrium constant approach.

In the heat and solute movement submodels, the conductivity and diffusion-dispersion coefficients were not dependent on the relative concentration of the parameter being simulated. In the case of infiltration, however, diffusivity and hydraulic conductivity are moisture dependent. To simulate the moisture movement between compartments, an "average" moisture content is determined for the gradient information. In this submodel the average is actually a weighted average to take into account the nonlinear diffusivity-hydraulic conductivity versus moisture content relationships. The flow between layers is thus the average diffusivity times the moisture content gradient plus the average hydraulic conductivity. The overall procedure is to first establish the initial and boundary (inflow) conditions. Then diffusivity and conductivity are calculated for each layer yielding the interlayer moisture movement. Net moisture content change and the input water are routed through the compartments by successively computing-adjusting until a stable mass balance is achieved or until changes from iteration to iteration are small.

GENERAL:

Although the model is detailed in the reference, a potential user is still left with a considerable effort to integrate the parts into a useable program. Fortran users will be able to develop such models with about as much effort.

MODEL: D-6

REFERENCES:

Frissel, M. J. and P. Reiniger. 1974. Simulation of accumulation and leaching in soils. Centre for Agricultural Publishing and Documentation, Wageningen, The Netherlands. pp. 70-84.

MODEL SCOPE:

Simulation is of diffusion, dispersion, adsorption-desorption, mass transport, and volatilization of herbicides in a homogeneous soil profile. Output includes the time and spatial distribution of the herbicides in the soil system.

INPUT REQUIREMENTS:

Two options are available: (1) instantaneous equilibrium (no adsorption); and (2) noninstantaneous equilibrium (adsorption-desorption). Both model options require volumetric moisture contents, bulk density, gas and liquid phase fractions, distribution ratios (soil/water, water/gas), soil profile depth, diffusion coefficient for gaseous phase, surface flux and concentration, and first-order decomposition rate coefficients for the herbicides. The noninstantaneous option also requires adsorption-desorption rates and water system diffusion rates.

SPATIAL AND TIME SCALES:

Simulation is of one-dimensional analysis of a one meter unsaturated soil profile. Calculations are presented at intervals specified by the user in hours or days.

COMPUTER CODE STRUCTURE:

CSMP

BASIC MATHEMATICAL APPROACH:

The flux of the herbicides due to water movement is described basically by the compartment modeling approach noted in other CSMP models. For the instantaneous equilibrium model, herbicides migrate in both the water and gaseous phases (only diffusion flux for the gaseous phase). Decomposition of the herbicide is a first-order reaction based on a decay rate. The analysis describes the convection and diffusion flux in the water phase and the diffusion flux in the gaseous phase. In the noninstantaneous equilibrium model, a linear adsorption reaction is assumed and added to the instantaneous equilibrium approach.

GENERAL:

The mathematics for the herbicide models are well defined in the reference. The models are listed in the reference. Field verification is not reported.

MODEL: D-7

REFERENCES:

Frissel, M. J. and P. Reiniger. 1974. Simulation of accumulation and leaching in soils. Centre for Agricultural Publishing and Documentation, Wageningen, The Netherlands. pp. 54-69.

MODEL SCOPE:

Simulation of diffusion, dispersion, and mass transport of Na^+, K^+, Ca^{++}, and Mg^{++} in soils. Model considers nonlinear adsorption-desorption. Output includes the time and spatial distribution of the salinity cations in the soil solute, adsorbed phase, and in deep percolation. The soil is considered homogeneous.

INPUT REQUIREMENTS:

Input consists of depth distributed and exchangeable solution Na^+, K^+, Mg^{++}, Ca^{++}, moisture content, Na^+/K^+, Ca^{++}/Mg^{++}, and adsorbed cation fraction/cation exchange capacity ratios, inflow rates and concentrations, fixed K^+ and fixation and release rates.

SPATIAL AND TIME SCALES:

Spatial scale is a one-dimensional analysis of a one meter or so depth of unsaturated soil. Calculations are reported in hours.

COMPUTER CODE STRUCTURE:

CSMP

BASIC MATHEMATICAL APPROACH:

The diffusion, dispersion, and mass transport are simulated by the CSMP compartmental model described previously. In addition, the cation exchange and potassium fixation are included to adjust the transport results. The exchange reaction is assumed to occur instantaneously. A Gapon equation, along with nonlinear functions (Vanselow), are incorporated, but the principal approach is one developed by the authors. Potassium fixation is a first-order reaction depending on relative concentration in solution and on the soil.

GENERAL:

More detail concerning the exchange processes is left to the interested reader. The input can be time distributed, but it is not clear how the moisture is redistributed since moisture content-conductivity relationships are not included. Program is listed in the cited reference.

MODEL: D-8

REFERENCES:

Frissel, M. J. and P. Reiniger. 1974. Simulation of accumulation and leaching in soils. Centre for Agricultural Publishing and Documentation, Wageningen, The Netherlands. pp. 12-20.

MODEL SCOPE:

Simulation of diffusion, dispersion, and mass transport of completely soluable compounds in the soil solute. Output includes the time and spatial distribution of the solute concentration and deep percolation. The soil is considered homogeneous.

INPUT REQUIREMENTS:

Input to the model includes depth of soil profile, number of compartmental soil layers, surface flux and inflow concentration, diffusion constant, anion exclusion ratio, initial moisture content, tortuosity and dispersion coefficients with soil depth, output frequency, and initial distribution of solutes.

SPATIAL AND TIME SCALE:

The spatial scale is an approximately one meter, one-dimensional view of an unsaturated soil profile. Calculation times are on the order of minutes with output printed at selected aggregate intervals of hours.

COMPUTER CODE STRUCTURE:

CSMP

BASIC MATHEMATICAL APPROACH:

The soil profile is divided into 40 compartments or layers with initial conditions defined in each layer. The diffusion coefficient for the boundary between two layers is computed using mean values of moisture content, tortuosity, and dispersion values. Diffusion rates are based on Fick's Law which calculates an average concentration gradient between layers and multiplies it by the diffusion coefficient to arrive at the flow. Mass flow is also based on average concentration and moisture flow rates. In this model, water flux is based on a steady-state infiltration.

The basic mathematical approach involves first calculating the movement rates between compartments. The rate of change in compartmental solute concentration is then computed and integrated using a standard CSMP semi-parallel method such as a fourth order Runge-Kutta method. The rates are recomputed and the iteration repeated until the compartment concentrations have stabilized.

GENERAL:

The program is set up for tritiated water. For other anions (Cl^-, NO_3^-), the rates are multiplied by the exclusion ratio. Code is presented in the cited reference. Verification is not reported.

MODEL: D-9

REFERENCES:

Hagin, J. and A. Amberger. 1974. Contribution of fertilizers and manures to the N- and P-load of waters, a computer simulation model. Report to the Deutsche Forschung Gemeinschaff. January. 123 pp.

MODEL SCOPE:

This detailed simulation model addresses the conditions which induce nitrate and phosphate pollution of receiving waters by fertilizers and animal wastes. The model evaluates the short term chemical, microbiological, and physical processes in the soil and then aggregates these results in the prediction of longer term outflow of nitrates and phosphates from the system. Nitrogen is assumed to originate as NO_3^-, NH_4^+, and organic material having differing C:N ratios. Simulation of subsequent nitrogen transformations include mineralization of organic-N to NH_4^+, nitrification of NH_4^+ to NO_3^- (assumed to occur in top 10 cm of the soil), and denitrification. Also included are the transport and plant uptake of NO_3^-. Phosphate is added to the soil surface and then moves through soil erosion. Model does not have either input dump or error flag systems. Input is accomplished by internally punched statements.

The nitrogen model is divided into the following sections: (1) water movement; (2) heat movement; (3) ammonification of organic-N; (4) oxidation of ammonium; (5) oxygen movement; (6) denitrification; and (7) nitrate movement.

The nitrogen model output includes hard copy plotting routines to present water content versus depth at different times, nitrate profiles, surface temperature profiles, cumulative plant uptake of nitrate, oxygen profiles, and total nitrate present.

The phosphate model consists of a section on water flow and one for soil detachment, transport, and deposition. Graphical output includes phosphorous erosion and sedimentation along field slope or outflow.

INPUT REQUIREMENTS:

The nitrogen model consists of 7 sections. Section 1, Water Movement, input includes rainfall and irrigation duration and intensities, class A pan evaporation, crop coefficients, soil hydraulic conductivity versus moisture content, conductivity at soil-atmosphere interface and various soil segments, diffusivity in various soil segments, depths and number of homogeneous soil layers, initial soil moisture conditions, and various root distribution and strength data.

Section 2, Heat Movement Data, includes air temperature, heat transfer coefficients, capacities, and initial conditions, and temperature of irrigation or rain water.

Section 3, Ammonification of organic nitrogen, requires the rate versus pH, temperature, and moisture dependent coefficients, percent organic matter added to soil as cellulose and other forms, immobilization-mineralization rates for Lignin, hemicellulose, sucrose, and cellulose, and additions or initial amounts of NO_3-N.

Section 4, Oxidation of Ammonium, input involves applied NH_4^+, relative mineral composition of soil and soil surface layers, soil material density, initial NO_3^- distribution, available nitrification bacteria, surface layer nitrification rate constants and coefficients, soil pH and temperature.

Section 5, Oxygen Movement, data include aerobic respiration rates, initial oxygen content in water throughout profile, and various other coefficients such as diffusion relationships.

Section 6, Denitrification, input includes carbon percentage of existing and added materials, denitrification rate coefficients and constants, and various initial conditions.

Section 7, Nitrate Movement, analysis requires input from previous sections, plus initial nitrate distributions, and diffusion and dispersion factors. Additional tortuosity and root uptake coefficients are also required.

These are by no means an exhaustive list and some misinterpretation of the code may result in listing an input where the actual data is computed.

For the phosphate part of the model, the water movement section requires geometries of soil subdivisions, rain and irrigation durations and intensities, surface hydraulic parameters, soil infiltration rates, porosities, and erosive parameters, slope of surface, etc. The second section requires data describing added nitrogen and phosphorus.

TIME AND SPATIAL SCALES:

Simulation is of a single or representation site on an irrigated or rain fed field. Time increments vary somewhat in the model from an almost continuous system for nitrogen transformation to daily events for irrigation or precipitation to weekly periods for parts of the evapotranspiration reactions. In general, the time scale is approximately a daily breakdown of the irrigation season. Model is one-dimensional.

COMPUTER CODE STRUCTURE:

CSMP

BASIC MATHEMATICAL APPROACH:

(1) Water Movement. Water is added to the upper soil layer through either daily inputs of precipitation or irrigation. Transpiration is determined with class A pan data multiplied by plant growth coefficients. The uptake by the roots represented by the transpiration is based on the

assumption that the uptake is proportional to the transpiration rates and distributed between soil layers according to relative root activity. A limit of 20 atmospheres is set on the moisture withdrawal in a layer. Water loss through soil surface evaporation is simulated for flooding, no-flooding, irrigation, and no-irrigation. Under no-flooding, no-irrigation, the evaporation is actually the difference between evapotranspiration as computed using pan data and transpiration. If the upward flow of water by diffusion is less than the previous difference, the evaporation is set at the smaller value. In the flooding case, the evaporation is equated to the class A pan values but for irrigation the corresponding value is assumed to be some minimal value.

(2) Heat Movement. The temperature of each soil layer is predicted by dividing the volumetric heat content by the volumetric heat capacity. Heat into and out of each layer due to moisture movement and transpiration is determined by multiplying flow rates by temperature. Heat conduction between layers is determined by multiplying the average heat conductivity of the two adjacent layers by the temperature gradient between layers.

(3) Ammonification of Organic-N. Mineralization and immobilization of nitrogen is assumed to occur in the upper 10 cm of the soil in a first-order reaction in which the mineralization rate is proportional to the available organic N. A distinction is made in organic materials according to their most common carbohydrate, lignin, cellulose, hemicellulose, and sucrose. The C:N ratios delineating the two processes vary with the carbohydrate. It should also be noted that additional reactions such as humification, the pH and moisture effects, and lignin inhibition are also considered.

(4) Oxidation of Ammonium. The nitrification rate equation used in this model is a first-order sigmoid curve. Only soil pH is evaluated directly in the model; temperature, moisture, and oxygen concentrations are assumed at their optimum values. The influence for each of these parameters is derived from literature reports.

(5) Oxygen Movement. Oxygen diffusion is modeled with Fick's second law by assuming simultaneous diffusion in both air and water in the soil. It is also assumed that instantaneous equilibrium between gaseous and dissolved oxygen occurs at any soil depth. Oxygen utilized in the oxidation of ammonium and organic carbon is also evaluated. This part of the model is one of the more complex included in the simulation. The reader is directed to the reference for specific details regarding definition of the diffusion coefficients, interlayer transfer, and consumption by organic carbon and ammonium processes.

(6) Denitrification. Probably the least developed of the nitrogen transformation simulations is denitrification. Hagin and Amberger (1974) treat the process as a first-order reaction with a rate coefficient determined by multiplying coefficients for temperature, pH, available organic matter, and oxygen-moisture.

(7) Nitrate Transport and Uptake. Nitrate is assumed to occur in the profile as an inflow with irrigation water, nitrification in the first soil layer, and as applied fertilizers. Nitrate losses consist of deep percolation, plant uptake and denitrification. Interlayer migration occurs either by diffusion or mass flow. Diffusion is proportional to the concentration gradient between layers and inversely proportional to the distance between layers. Mass flow occurs with the moisture movement but is adjusted with a dispersion coefficient. The uptake of nitrate is calculated by multiplying the volume of moisture uptake by the soil water nitrate concentration (with unit conversions) but limited to some upper limit. Finally, nitrates can accumulate in a soil layer or be leached depending on a mass balance computation.

For the transport of phosphates in surface runoff and erosion, the upper soil layer is assumed sufficiently permeable that runoff would not occur until it is saturated. The depth of surface runoff is computed much like the surface irrigation advance analyses, i.e., a mass balance between the surface and infiltrated moisture. The erosion mechanism includes soil detachment by rainfall and runoff and transport capacities of both rainfall and runoff. The individual processes utilized in this phase of the model are presented in the technical literature.

GENERAL:

This is one of the more detailed treatments of the nitrogen-phosphate system in irrigated agriculture, but most of the model is developed from data published in the literature. The calculations presented are likewise based on reported data. Consequently, the "general" nature of the model may remain somewhat in question until it is applied and verified against field data taken at one location. It should be useful in evaluating the interrelationship in this complex system and is therefore primarily a research tool. The code is included in the cited reference.

MODEL: D-10

REFERENCES:

Hillel, D. 1977. Computer Simulation of Soil Water Dynamics. International Development Research Centre, Ottawa, Canada. pp. 131-134.

MODEL SCOPE:

Simulation is of the water budget and noninteracting solute transport in the unsaturated crop root zone. Model includes root extraction, root growth, and the spatial-time distributed flux of water and solute.

INPUT REQUIREMENTS:

Parameters are specified defining the geometry of the soil and root system, hydraulic properties of soil and roots, daily transpiration demand, hydrodynamic dispersion coefficient, and water potential at the plant crown. Tables of relative root length in the vertical profile, initial moisture and solute conditions, suction, wetness and conductivity relationships, and wetness-tortuosity relationships are specified.

TIME AND SPATIAL SCALES:

This model is a one-dimensional treatment of the unsaturated root zone determined for one second intervals aggregated to hourly and daily summaries.

COMPUTER CODE STRUCTURE:

CSMP

BASIC MATHEMATICAL APPROACH:

The compartmentalized soil system is assumed to be in a state similar to post-irrigation or post-rainfall by specifying the initial distribution of soil moisture. Moisture movement between layers is based on calculating an average hydraulic gradient and conductivity between soil layers or compartments. Then intercompartmental flux is used iteratively to recompute moisture content.

The uptake segment of the model involving developed or growing root systems is based on distributing the transpiration through the soil profile. The relative extraction in a compartment is the ratio of the difference between the moisture potential in the compartment and the crown potential to the sum of the hydraulic resistance of the soil (conductivity x length of flow path) and the compartment's root resistance. The crown potential is identified by successive approximation. If root birth and extension are considered, exponential functions are used to simulate them so the rooting pattern can be updated at each iteration.

GENERAL:

Verification trials are not reported although results are presented illustrating the model results. The code is listed in the reference.

MODEL: D-11

REFERENCES:

Margheim, G.A., 1967. Predicting the quality of irrigation return flows. Unpublished M.S. Thesis, Civil Engineering Department, Colorado State University, Fort Collins, Colorado, December. 57 pp.

MODEL SCOPE:

Simulation is of the salinity constituents in flows entering the groundwater basin under irrigated croplands. Parameters include the concentrations of Ca^{++}, Mg^{++}, Na^{+}, and $SO_4^{=}$ in the flows entering the water table from deep percolation. The computer code does not contain an input dump or a printing of intermediate results, but does contain partial error flags for iteration limitations.

INPUT PARAMETERS:

No control parameters are utilized. Input data include the irrigation water concentrations of Ca^{++}, Mg^{++}, Na^{+}, Cl^{-}, and $SO_4^{=}$, and the concentrations of exchangeable Na^{+}, Ca^{++}, and Mg^{++} in the soil. Input also requires concentrations of soluable Mg^{++}, Na^{+}, Ca^{++}, and $SO_4^{=}$ in the soil, solubility product of gypsum, and cation exchange constants for homovalent and monovalent-divalent exchange equations.

SPATIAL AND TIME SCALES:

Analyses are at a single or representative site in an irrigated field (accomplished by assuming uniform irrigation water applications). Steady-state moisture flux is assumed so time scale is set by user. However, an irrigation interval is generally selected.

COMPUTER CODE STRUCTURE:

Internal program linkage is facilitated by subroutines with data and results transferred through call statements. Program can be easily adapted to other computer systems since tape and disc functions are not performed. Core requirements are less than 40 k bytes while execution times are not known (probably 10-15 seconds per run). Model is programmed for CDC 6400 using Fortran IV language.

BASIC MATHEMATICAL APPROACH:

Under assumptions that gypsum is the only slightly soluble salt present in the soil system, the model first computes the ion concentrations in water percolating below the root zone and then the concentration of water intercepted by a drainage system. Effects of evapotranspiration are not directly considered in the soil chemistry phase. Computations in the soil chemistry phase involve the following iterative procedures controlled by iteration to iteration changes in calcium concentrations. A volume of irrigation water equal to the stored soil moisture volume is equilibrated with the soil-$CaSO_4$

system using the Gapon equation for exchange processes, and the Debye-Huckel gypsum solubility relations for solution equilibrium. The iterative procedure is repeated once the successive approximation procedure has converged for other volumes of irrigation water until the desired leaching is accomplished. Then, using a drainage equation developed by R.E. Glover, the volume of return flow is computed. The model assumes groundwater quality is poorer than deep percolation and mixing does not occur. An interface is thereby formulated from which the relative displacement is determined to arrive at the outflow mixture.

GENERAL:

Code is available in reference cited above. However, code is not documented nor verified against field data.

MODEL: D-12

REFERENCES:

Childs, S. W., and R. S. Hanks. 1975. Model of soil salinity effects on crop growth. Soil Sci. Soc. Amer. Proc., 39:617-622.

Nimah, M. D., and R. J. Hanks. 1973. Model for estimating soil water, plant, and atmospheric interrelations: I. Description and Sensitivity, and II. Field test of model. Soil Sci. Soc. Amer. Proc., 37:522-527 and 37:528-532.

Melamed, J. D., R. J. Hanks, and L. S. Willardson. 1977. Model of salt flow in soil with a source-sink term. Soil Sci. Soc. Amer. Proc., 41:29-33.

MODEL SCOPE:

The model described here is actually the result of several individual models. Nimah and Hanks (1973) added a plant root extraction system to an earlier one-dimensional moisture flow model. Childs and Hanks (1975) modified the Nimah and Hanks (1973) model for crop growth, salt flow, and irrigation uniformity. Then, the "Dutt Model" described herein by Dutt et al. (1972) and a simple source-sink model to account for chemical reactions were added. The simpler salt system was added to the water model by Melamed et al. (1977). Because the more complex Dutt model is described elsewhere, the version will not be detailed here.

The model simulates the one-dimensional flow of water in the transient, unsaturated soil profile including the spatial distribution of root uptake in response to surface evapotranspiration demand. Salts added to the system in the irrigation water or that exist in the solid form in the soil structure are transported through the system to the groundwater below. Dissolution and precipitation of salts in the root zone are simulated as a source-sink process rather than by chemical equilibrium. Ionic exchange and biological transformations are neglected. Output describes the spatial and time distributed water-salt system including evapotranspiration.

INPUT REQUIREMENTS:

The primary data necessary for the soil moisture flux are the hydraulic conductivity-water content and pressure head-water content relations, air dry and saturated moisture contents, root water potential below which wilting occurs, depth distributed root distribution, initial moisture distribution, potential evapotranspiration at the surface and water inputs (irrigation or rainfall), osmotic potential of the irrigation water and of soil (depth distributed), the presence of a lower boundary water table, and crop cover. The salinity simulation requires the electrical conductivity of the irrigation water and solid soil salts, diffusion and dispersion coefficients, and initial solute distribution (electrical conductivity).

TIME AND SPATIAL SCALES:

The model is a one-dimensional analysis of the root zone. Time scales vary in length from an irrigation interval to several years.

COMPUTER CODE STRUCTURE:

Programs are written in Fortran IV with common and call data transfer to subroutines. Execution time depends on the length of the real time simulation. Core requirements appear moderate (50-70 k bytes).

BASIC MATHEMATICAL APPROACH:

The model involves a moisture flow simulation, a salt transport system, and a simulation of the dissolution-precipitation processes (source-sink term). The moisture flow equation is the moisture content form of the unsteady flow equation developed by writing Darcy's Law and mass conservation equations in one dimension. This primary flow equation is modified by the inclusion of a root extraction term and solved with a implicit finite difference technique. The essential features of the root extraction term are described by Nimah and Hanks (1973). (See also the model of Feddes and Zaraday, 1977.) Flow to the roots is based on the difference between the root potential plus root resistance and the combined soil water and osmotic potentials. This value is then multiplied by the hydraulic conductivity and a depth distributed rooting pattern. The root potential is determined by maximizing transpiration as was the case in the model by Feddes and Zaraday (1977) (which was based on this model).

The solute transport relationships are based on the equation of Bresler (1973) which includes diffusion and hydrodynamic dispersion. This equation is solved using a tridiagonal matrix solution of a Crank-Nicholson finite difference method.

The source-sink term accounting for precipitation and dissolution of salts is an on-off linear equation based on the difference the salinity concentration of the soil solution and a value at which precipitation will occur. The equilibrium concentration must be evaluated in the field.

GENERAL:

The model which has been calibrated against field data shows good predictive agreement with observed field data once calibrated. The code should be requested from its authors.

MODEL: D-13

REFERENCES:

Smajstrla, A.G., D.L. Reddell, and E.A. Hiler. 1974. Simulation of miscible displacement in soils. Paper 74-2015 presented at the Annual Meeting of ASAE, Stillwater, Oklahoma. June. 31 pp.

MODEL SCOPE:

Simulation is of vertical miscible displacement of noninteracting solutes in unsaturated, homogeneous, isotropic soils. Analysis includes the effects of convection, ionic diffusion, and mechanical dispersion. Output describes the time and depth distributed values of water content and solute concentrations during an infiltration event.

INPUT REQUIREMENTS:

The first group of input data includes the number of soil layers being considered, number of moving points, a control for infiltration versus redistribution phases, number of points in the capillary pressure versus water content table and the number of points in the water content-hydraulic conductivity table. Then the pressure versus water content and water content versus hydraulic conductivity tables are read in. Next, the grid characteristics are defined (initial moisture and solute state, thickness, and location of moving points). Following these data, the saturation moisture content, saturated hydraulic conductivity, surface pressure during infiltration, total intake of water and salt, salt concentrations and tracer depths allowed, simulation time and time infiltration stops, output intervals, and several increment values not specified are assigned.

SPATIAL AND TIME SCALES:

Model evaluates the one-dimensional transport of soil solutes in the unsaturated zone, presumably in an irrigated situation. The overall time scale is the infiltration-redistribution period, something on the order of one to five days. Time intervals on the order of tenths of hours are used to solve the flow equations.

COMPUTER CODE STRUCTURE:

The computer code is written in Fortran IV for IBM 360/65 computer but appears readily adaptable to most other kinds as well. A main program serves only to control the order of calculations by sequentially addressing various subroutines. Data is maintained in common blocks. Core storage requirements do not appear to exceed 50-70 k bytes but execution time would be highly variable depending on the length of simulation and resolution in the grid system.

BASIC MATHEMATICAL APPROACH:

This analysis assumes a homogeneous, isotropic soil with respect to both physical and hydraulic properties. In addition, it is assumed that head versus moisture content and hydraulic conductivity are single valued functions, ions are noninteracting and conservative, and the viscosity of the water is constant. The nonsteady Darcy equation and the convective-dispersive solute transport equations are solved simultaneously. The evaluation of both convective and dispersive processes is made using the method of characteristics which effectively separates the two processes and thereby eliminates numerical dispersion. Solution of the moisture flow equation is accomplished with an explicit finite difference technique, as was the solution for dispersion effects. A system of moving points within the grid was used with the method of characteristics for calculating the moving position of the solute. A more detailed, description of the numerical procedure can be abstracted from the reference cited above.

GENERAL:

The program is well written and documented. Although the analysis would be limited to the conservative ions like chloride, the results would be useful in predicting selected aspects of the irrigation return flow system, for example, leaching fractions. Code is listed in the cited reference.

APPENDIX E

DESCRIPTION OF WATERSHED HYDROLOGY MODELS

MODEL: E-1

REFERENCES:

Hillel, D. 1977. Computer Simulation of Soil-Water Dynamics. International Development Research Centre, Ottawa, Canada. pp. 155-198.

MODEL SCOPE:

Simulation is of the hydrology of a sloping agricultural field. Processes modeled include precipitation, infiltration, runoff, evaporation, redistribution, deep percolation, capillary rise from the water table, and groundwater drainage. Plant uptake and transpiration are not included. Output depicts the time and spatial distribution of water in the system.

INPUT REQUIREMENTS:

The geometry of the system is defined by stating the number of columns, number of layers per column, width of each column, and vertical dimensioning. Initial conditions such as saturated hydraulic conductivity and initial moisture distributions are detailed. The runoff hydraulic parameters are input, including roughness factors for the Manning's equation and surface slope. Boundary conditions are defined to depict the potential evaporation rate, water table elevation at its outflow to the drain and rainfall inputs. As in other unsaturated soil models, the relationships between water content, hydraulic conductivity, and suction must be known.

TIME AND SPATIAL SCALES:

The scale is a two-dimensional evaluation of a field sized system extending vertically to an impervious layer. The principal event is the period immediately preceding and shortly after a rainfall (until equilibrium conditions occur).

COMPUTER CODE STRUCTURE:

CSMP

BASIC MATHEMATICAL APPROACH:

Water added to the soil surface is divided into infiltration, surface storage and runoff. Infiltration is calculated by dividing the vertical unsaturated soil profile into layers and then routing flows through it using an iterative computation of contents, gradients, rates, and new contents. Runoff is handled by dividing the field into a number of vertical columns and then routing the surface water down slope with a successive kinematic wave equation. At the bottom of the slope the time distributed runoff is yielded by the last computations. In each column, the infiltration crossing the last compartment in the unsaturated zone is the inflow to the groundwater basin. A water table height increase is distributed through each column and then the saturated soil properties along with hydraulic gradients are used to calculate a lateral groundwater flow for the bottom of the slope.

GENERAL:

No field verification is presented. Code is listed in cited reference.

MODEL: E-2

REFERENCES:

Makkink, G. F. and H. D. J. Van Heemst. 1975. Simulation of the water balance of arable land and pastures. Centre for Agricultural Publishing and Documentation, Wageningen, The Netherlands. 79 pp.

MODEL SCOPE:

Simulation is of water movement and storage in a cropped field and the saturated-unsaturated soil beneath. The processes modeled include snow precipitation and melt, canopy interception and evaporation, soil surface evaporation and infiltration, unsaturated and saturated flow, evapotranspiration, micellar flow and plant withdrawal and hydration-dehydration. Output involves the time and spatial distribution of water in the system.

INPUT REQUIREMENTS:

The data listed as required input include the date of the last balance period and the current date, global and extraterrestrial solar radiation, a "place factor", air and dew point temperatures, relative humidity, wind speed, crop height, and depth of root zone, all for each day of the analysis. However, a number of data not listed as input are required nevertheless. For instance, the conductivity and moisture versus suction relationship, initial conditions, infiltration, and soil and crop characteristics are internal to the program as DATA statements.

SPATIAL AND TIME SCALES:

The analysis is of a large crop area, but the evaluation is made at one vertical "average" location. Time increments of 0.2 days are used in the calculation with output based on daily intervals. Model is one-dimensional and steady-state.

COMPUTER CODE STRUCTURE:

Code is written in Fortran IV for the CDC series computers. A main program with common linked subroutines and functions comprise the basic code structure. Although neither core nor time requirements are discussed, they are obviously small enough for most computers.

BASIC MATHEMATICAL APPROACH:

The plant-soil system is divided into "compartments" representing the various forms of moisture storage in the system. The computational system involves an iterative evaluation of compartment storage, the rate of moisture movement between compartments, and the calculation of contents (CONTENT at time t = CONTENT at time t-1 + RATE times Delta Time). The storage compartments include snow (existing as solid precipitation or heavy frost and flowing in the system by evaporation and melting), adhering water which stems from canopy interception (this moisture evaporates, drops into pools, or drops onto and infiltrates unsaturated soil). Pools filled with precipitation at rates greater than the saturated hydraulic conductivity of the soil (released from pools by evaporation and infiltration), the unsaturated soil profile (transmitting water to the saturated zone below or to the atmosphere above through transpiration and evaporation), the saturated zone (venting to transpiration, groundwater flow, water table storage changes, and flow to the unsaturated region through capillary use) and micellar water taken up by and stored in the clay structure. Subsets of the mass balance in the unsaturated zone are developed for the upper soil profile contributing to evaporation and the region of plant uptake. There are also storage balances for the moisture stored above and below 16 atm and field capacity, respectively. The basic rate processes are evapotranspiration and soil moisture redistribution. Evaporation and transpiration are computed with modified forms of the Penman equation. Unsaturated flow occurs when the soil moisture level exceeds field capacity.

GENERAL:

Although this model has many aspects of a general nature, its existing format is entirely site specific to the case studies it was validated against. To apply this model to other situations, much more data are needed. The code is presented in the reference cited above.

APPENDIX F

DESCRIPTION OF WATERSHED HYDRO-QUALITY MODELS

MODEL: F-1

REFERENCES:

Dutt, S.R., M.S. Shaffer, and W.S. Moore, 1972. Computer simulation model of dynamic bio-physicochemical processes in soils. Technical Bulletin 196, Agricultural Experiment Station, University of Arizona, Tucson, Arizona. October. 101 pp.

Shaffer, M.S., R.W. Ribbens, and C.W. Huntley. 1977. Prediction of mineral quality of irrigation return flow, Volume V. Detailed return flow salinity and nutrient simulation model. EPA-600/2-77-179e. Robert S. Kerr Environmental Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Ada, Oklahoma. August. 228 pp.

MODEL SCOPE:

This model simulates chemical and physical processes associated with agricultural lands drained by subsurface drainage systems. Basic input data involves the field application of irrigation or precipitation with associated salts and nitrogen nutrients. Model output is the prediction of drainage quality with evaluations at intermediate points in the plant-soil-aquifer system. Program includes intermediate output and various error flags.

INPUT DATA:

This is a very large computer model well documented by Shaffer, et al. (1977). As a consequence, the input requirements are elaborate. The following input data summary is given by Shaffer, et al., (1977):

(1) Drainage parameters: drain spacing and depth, depth to impermeable barrier, envelope size, saturated hydraulic conductivity, porosity, and specific yield or storage coefficients;

(2) Unsaturated flow parameters: the hydraulic conductivity versus moisture content function, and pressure head versus moisture content relations;

(3) Soil chemistry data: meq/l of Ca^{++}, Mg^{++}, Na^{+}, $CO_3^{=}$, HCO_3^{-}, Cl^{-}, $SO_4^{=}$, NH_4^{+}, NO_3^{-}, and urea in soil extract, pH, cation exchange capacity, gypsum content, presence of lime, bulk density, organic

nitrogen, carbon-nitrogen ratio, and the nitrifier population-salt response relationship;

(4) Crop information: rooting depth and distributions, evapotranspiration rates as read in or calculated using an irrigation scheduling program, and plant uptake of nitrogen;

(5) Water application data: irrigation schedules and amounts (or precipitation amounts and timing) and an effective precipitation relationship;

(6) Fertilizer data: fertilization schedules, amounts of NO_3^-, NH_4^+, Urea, Ca^{++}, $SO_4^=$, and $CO_3^=$, application depth and organic nitrogen-plowed in with corresponding C-N ratio, and application ratio;

(7) Irrigation water analyses: concentrations of NH_4^+, NO_3^-, Ca^{++}, Na^+, Mg^{++}, HCO_3^-, $CO_3^=$, Cl^-, and $SO_4^=$; and

(8) Miscellaneous soils data: soil temperature and coefficients relating to nitrification and denitrification.

SPATIAL AND TIME SCALE:

The spatial scale is a two-dimensional evaluation of the vertical region from the soil surface to the drainage system. Time scales are mixed depending on the calculation being made. Time varies from fractions of a day to an irrigation interval and even up to an irrigation season. The model is transient in nature.

COMPUTER CODE STRUCTURE:

The primary code structure is in a main program-subroutine format utilizing common, call, and tape file data transfer. The size of this model requires extensive use of overlay systems if the entire package is used. Consequently, core requirements are only 140-150 k bytes at any instant. Time for execution varies from one to two minutes up to several minutes depending on the scope of the job. Although the basic program language is Fortran IV, this model is not easily adapted in its entirety. Except for some planning use by the Bureau of Reclamation, this is primarily a research tool and not applicable by most planning groups.

BASIC MATHEMATICAL APPROACH:

This model is comprised of individual models which extend across several disciplines. Consequently, there is more likely to be more interest in the various submodels rather than the total package. The program is linked together with detailed overlay systems and numerous by-pass options provide substantial flexibility. The interested user can find excellent explanatory comments in the references noted above. However, to identify the model's basic characteristics, this section will be divided by major submodels.

Irrigation scheduling. Unlike the irrigation scheduling program available to schedule and update irrigations, this model predicts irrigation schedules and amounts using historical data exclusively. Based on geographical data, solar radiation, and temperature, the program first computes potential evapotranspiration for alfalfa using the Jensen-Haise equation. Adjustments are made for seven other crops using standard growth stage coefficients. Then, a simple mass balance of the root zone is developed. Soil moisture is allowed to be depleted to an "allowable moisture depletion" before an irrigation is scheduled. Coefficients for various irrigation efficiency and losses produce deep percolation and surface runoff estimates. The output from the model is recorded on cards punched for subsequent use in the unsaturated moisture-chemistry models (infiltration) and the drainage calculation (deep percolation).

Soil moisture movement. The unsaturated flow submodel is a finite difference simulation of the transient moisture flow equation in one dimension. Hydraulic conductivity is taken as a function of moisture content as is pressure head. Simulation includes infiltration, redistribution, drainage, and plant uptake. Plant uptake is determined from information of total uptake which is distributed throughout the soil profile in proportion to an average root distribution.

Unsaturated soil chemistry. The complex soil-water system is simulated from a chemical-biological standpoint by a group of subroutines designated as the unsaturated chemistry program. The program has two primary components: (1) simulation of the soil nitrogen system; and (2) the soil salinity series. This model is the basic programming package reported by Dutt, et al. (1972).

The nitrogen phase of the program considers urea hydrolysis, nitrification of NH_4^+-N, net mineralization-immobilization of both organic-N and NH_4^+-N, immobilization of NO_3^--N, plant uptake of NH_4^+-N and NO_3^--N, and denitrification. In addition, the NH_4^+-N reaction in the cation exchange system is considered. With the exception of the cation exchange process, the nitrogen simulation assumes a first-order kinetic approach using regression functions for the transformation rates. Denitrification is evaluated using zero-order kinetics. Nitrogen uptake may be evaluated by either of two methods. First, the user may specify total N uptake and root distribution which yield the plant N uptake in each soil segment per unit of time. In this case, the user specifies the fractions of NO_3^-, and NH_4^+ uptake. The second assumes uptake is proportional to water uptake. Output from these segments of the model predicts mass distribution of the various nitrogen components.

The salinity phase of the models evaluates ion exchange, solution-precipitation of gypsum and lime, formation of undissociated ion pairs, and transport of the soluble species (Ca^{++}, Mg^{++}, Cl^-, Na^+, etc.). Because these various reactions occur quickly, solution equilibria are used to describe the segments of the salinity system. The ion exchange and solution-dissolution of the slightly soluble salts are computed using standard approaches such as the Gibbs phase rule, Debye-Huckel theory, and Gapon equations. An iterative successive approximation procedure is used to determine the chemistry within the soil profile and in the deep percolation. The procedure involves (1) calculation of lime solubility; (2) calculation of gypsum solubility;

(3) undissociated $CaSO_4$ and $MgSO_4$ ion pair reaction; (4) Na^+-Ca^{++}, Mg^{++}-Ca^{++}, and Na^+-NH_4^+ ion exchange; and (5) evaluation of $CaCO_3$ dissociation.

The movement and distribution of water is either read in or produced by the unsaturated flow program. For the soluble ions, a mixing cell concept is used to simulate solute dispersion and movement. This assumes complete mixing occurs in each soil-time increment and that molecular diffusion is negligible.

Drainage Model (Dynamic Equilibrium). Flow moving below the crop root zone is routed to surface receiving waters via this drainage program. The model was designed to predict the response of a subsurface drainage system consisting of parallel, equally spaced tile drains, to deep percolation inputs. Principal outputs are the mid-space water table elevation and drain discharge. Deep percolation may be developed for the program through card read input or directly from the unsaturated flow model. The mathematical approach is the general Bureau of Reclamation drainage equations.

The water table shape is approximated as a fourth degree parabola which uses specific yield to compute instantaneous rises and declines in water table positions. Hooghoudt's equivalent depth is used to correct for near-drain convergence effects not treated by the Dupuit-Forchheimer assumptions. The Moody solutions are used to approximate these systems.

Drainage Model (steady-state). The general modeling system also includes a steady-state drainage system model based on potential theory to define stream tubes. An average deep percolation rate is computed from the values determined by the unsaturated flow program. A system of nodes are defined at which the infinite series mathematical solutions are computed. Under this approach, the flow velocities and travel times are estimated thereby yielding an estimate of the time required for a water volume to reach the drainage system. These data are determined for use in the saturated chemistry and drainage effluent chemistry parts of the program.

Saturated Chemistry Program. This program predicts the two-dimensional distribution of saturated flow chemistry below an irrigated field. The stream tube flows predicted by the steady-state drainage model along with chemical soil analysis serve as model input. Each stream tube is analyzed separately and is divided into segments of equal volumes. Flow is accumulated until it reaches the pore volume of a segment and then is moved by piston displacement. After each displacement, the solution is equilibrated with the solid and exchangeable phases. Lateral dispersion and diffusion are neglected since lateral and longitudinal mixing among stream tubes is not considered. Chemical transformations are identical to those in the unsaturated chemistry model except denitrification is simulated in the transition zone between unsaturated and saturated regions. The denitrification rate is assumed temperature dependent but not affected by substrate concentration. Above a "saturation level" the rates are assumed to be zero-order and below this level to be first-order. The aquifer profile is assumed to be homogeneous until the heterogeneous nature is computed through consideration of individual stream tubes.

Drain Effluent Prediction. This program takes the flow rates from the steady-state drainage analysis and its corresponding chemistry and aggregates each stream tube into a monthly drainage discharge. The salt load from the drainage system is thus determined by mixing and routing the flows in each stream tube.

GENERAL:

This modeling system is well documented, verified in field conditions, and available for broad use. However, the system itself is far larger than required by most research groups and far too complex for use by planning groups. Many possible uses can be made using individual segments listed above. Computer and data requirements are substantial. The modeling system is probably the largest, most exhaustive available as an integrated package. Code listings are available from the Bureau of Reclamation.

MODEL: F-2

REFERENCES:

Bureau of Reclamation. 1977. Prediction of mineral quality of irrigation return flow, Volume III, Simulation model of conjunctive use and water quality for a river system or basin. User's Manual. EPA-600/2-77-179c. Robert S. Kerr Environmental Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Ada, Oklahoma. August. 295 pp.

MODEL SCOPE:

Simulation is of the water and salinity impacts in a river basin resulting from urban, industrial, and agricultural water uses. Formulated as part of a need for evaluating irrigation return flows in a river system, the model is primarily oriented to this end. In addition to the mass balance of surface and groundwater in a river section, the model simulates reservoir operations, and a comparatively complex analysis of the soil salinity system. Program features both input dumps and error flags. Intermediate results are not presented.

INPUT REQUIREMENTS:

Control parameters are initially read in to completely dictate problem structures since enough flexibility has been added to allow simulation of river systems with a multitude of local conditions. Control parameters include division of system into segments (nodes), processes being simulated in each segment, node structure and labels, and time dimensions. Input data descriptive of local hydrochemical processes are input as follows: (1) aquifer volume and salinity; (2) reservoir conditions and operating rules; (3) sediment analyses; (4) irrigated soil chemical and hydraulic characteristics; (5) hydropower generation parameters; (6) discharge and chemistry of major surface and subsurface inflows; (7) demands by agricultural, municipal and industrial users; and (8) allocation of flows within an irrigation system.

SPATIAL AND TIME SCALES:

Simulation is of hydrochemical systems on a river basin scale or segment thereof. Time period utilized is one month at minimum scale to several years duration of simulation.

COMPUTER CODE STRUCTURE:

Internal program linkage is accomplished by subroutines and functions with both common and call statement data transfer (control parameters are generally passed in the call). Code is set up to read and write results as output or onto tape or disk systems. Approximate core and execution time requirements are 140 k bytes and 120 central processor seconds, respectively. Program language is Fortran.

BASIC MATHEMATICAL APPROACH:

The program utilizes an iterative scheme for balancing mass between "nodes" or subbasins comprising the area being analyzed. This model includes substantial simulation of reservoir and stream management. After initialization of the system, the various demands are compared with the available stream flow to determine if a shortage is occurring. If insufficient water is available in the river, a series of reservoir checks and manipulations are made to adjust flow if possible. Return flow volumes and chemistry are then computed and checked against initial assumptions. Iterations are repeated until mass balance is achieved.

Of particular interest in this review is the model segments describing the irrigation return flow system. Diversions are determined by computing the consumptive use (using the Penman equation) and then dividing by conveyance and farm irrigation efficiencies. Return flow is then the difference between demand and consumptive use. The chemical simulation of the soil profile is based on a simplified version of the model presented by Dutt, et al., 1972.

GENERAL:

Model is very complex in scope and therefore difficult to apply without some previous experience in hydrosalinity modeling on a large scale. However, the user manuals are excellent descriptions of the computer system and can be used to implement the model. This model has been used extensively by the Bureau of Reclamation in studies throughout the western United States. The code is available from the Bureau of Reclamation.

MODEL: F-3

REFERENCES:

Crawford, N. H. and A. S. Donigian. 1973. Pesticide transport and runoff model for agricultural lands. EPA-660/2-74-013, Office of Research and Development, U.S. Environmental Protection Agency, Washington, D.C. December. 317 pp.

Donigian, A.S. and N. H. Crawford. 1976. Modeling pesticide and nutrients on agricultural lands. EPA-600/2-76-043. Office of Research and Development, Environmental Research Laboratory, U.S. Environmental Protection Agency, Athens, Georgia. February. 211 pp.

MODEL SCOPE:

Simulation is of runoff, snow accumulations and melt, sediment loss, pesticide-soil interactions, and soil nutrient transformations. Analysis involves transport of pollutants from both surface and subsurface sources. The model is intended for watersheds up to two square miles in which in-channel processes and transformations can be neglected. Parameters simulated include mass transport of water, sediment, pesticides, nitrogen and phosphorus. The program is set up to operate in either a calibration or production mode. In general, the output includes water movements (runoff, infiltration, evapotranspiration, and storage), sediment transport, pesticide transport and transformation in various soil layers and in sediment, nutrient transformations in the soil profile, and leaching of nitrate. The only salinity parameter in this version of the model is chloride. Output can be controlled to intervals from every 5-15 minutes in the simulation to monthly summaries.

INPUT REQUIREMENTS:

Data necessary to operate the model can be divided into control, hydrologic, snow, sediment, pesticides, and nitrogen-phosphorus parameters. The control parameters include type of run, units, output interval, snow, pesticide, nutrient simulation options, input data checks, time intervals for calculations, watershed structure, and time limits. For the hydrology submodel, input includes soil moisture storage (capacity and initial), length, slope, roughness, intake, evaporation coefficients, and surface storage of watershed, groundwater return flow timing, and groundwater distribution and conditions. The snow accumulation-melt analysis requires a number of coefficients describing the energy balance description of the solid-liquid phase transformations, climatological parameters (radiation, temperature, wind), and topographic description of the watershed. To compute the sediment phases of the model, the user must supply crop cover, tillage effects (depth, timing, and fine deposits), soil depths and bulk densities, rainfall splash coefficients, overland flow exponent and wash-off coefficient, and the initial soil fines deposit. Pesticides are described using application timing, solubility, fixing capacity, coefficients in the Fruendlich adsorption/desorption equation, decay rate, and control coefficients noting how the pesticide is applied and whether or not a single-valued adsorption/desorption algorithm is to be used. Nitrogen and phosphorous simulation begins by first specifying time steps, number of fertilizer applications, and harvest dates. Then a series of nitrogen reaction rates for mineralization, immobilization, nitrification, denitrification, and uptake are input. Similar coefficients are needed for phosphorus analysis. Storage of nitrogen (in its various forms) and phosphorus is detailed by describing the adsorbed, dissolved, absorbed, and gaseous phases.

SPATIAL AND TIME SCALES:

Calculations are based on a 5 or 15 minute real time interval with results lumped in hourly, daily or monthly summaries. The spatial scale is of a 1-2 square mile agricultural watershed.

COMPUTER CODE STRUCTURE:

The basic code structure is one of a main program controlling the order and presentation of input, calculations, and output with subroutines encompassing specific submodel tasks. The code is written in Fortran IV and run on a IBM 360/67 computer but appears readily adaptable to other machines. The code is very lengthy and is best operated in compilation and production steps. The number of pages of output can be several hundred with even routine analysis. Neither core requirements nor execution times are noted, however, both are comparatively large on visual inspection.

BASIC MATHEMATICAL APPROACH:

This model is too large for a thorough description of the mathematical approach. Consequently, only a brief summary will be presented here with more detail left to the interested user. The code involves six primary subprograms: (1) MAIN which orders overall execution; (2) LANDS which simulates the hydrology and snow; (3) SEDT, the analysis of sediment, (4) ADSRB, the pesticide adsorption and removal program; (5) DEGRAD, pesticide degradation; and (6) NUTRNT, which is the simulation of nutrient transformation and removal.

The LANDS subprogram is derived from the Stanford Watershed Model presented in various publications. The hydrologic response of a watershed to inputs of precipitation and evaporation involves a water budgeting procedure which accounts for evapotranspiration, surface storage and retardance, infiltration, groundwater storage depletion and return flow, and overland flow.

The SEDT subprogram is a simulation of sheet and rill erosion involving the processes of particle detachment by rain drop impact and transport by overland flow. The particles detached during an interval are expressed as a power function of vegetal cover, precipitation, and a detachment coefficient. Overland transport is expressed as a power function of the detachment coefficient, initial volume of soil fines, and overland flow rate. Attempts have been made to include the effects of tillage operations by allowing the user to redefine initial volumes of detachable soil fines. Vegetal cover effects are specified monthly by the user with linear interpolation during the month.

The subprogram ADSRB is based on two alternatives. First, the standard single-valued Freundlich adsorption/ desorption isotherm is used to separate adsorbed and dissolved pesticide concentrations. The second approach involves a multiple valued adsorption/desorption process taken from the work of Davidson, et al. (1975) reported elsewhere in this writing.

The degradation and volatilization of pesticides are simulated in the subprogram DEGRAD. Volatilization is ignored in the model's present version and degradation is assumed to follow a first-order decay function.

The nutrient simulation model (NUTRNT) attempts to predict nitrogen and phosphorus losses due to erosion, surface washoff, leaching, and biological conversion. Phosphorus is assumed to exist as organic phosphorus, solid phosphate, dissolved phosphates, and phosphorus adsorbed by the plants. Transformations are all based on first-order kinetics (temperature dependent). Nitrogen processes (mineralization, immobilization, nitrification, denitrification, and uptake) are based on first-order kinetics using literature values of the coefficients. Ammonium adsorption/desorption is also included in the model. Solution of the coupled differential equations is accomplished with a simple Euler integration scheme.

GENERAL:

This model is currently being improved and modified for a more general use. The nutrient phases remain unverified at this time although the surface hydrology and pesticide portions are tested against actual field data. Code listing is presented in the reference.

MODEL: F-4

REFERENCES:

Dixon, N.P., D.W. Hendricks, A.L. Huber, and J.M. Bagley. 1970. Developing a hydro-quality simulation model. Report PRWG 67-1. Utah Water Research Laboratory, Logan, Utah. June. 193 pp.

MODEL SCOPE:

Simulation is of the electrical conductivity, dissolved oxygen, temperature, BOD, and coliform count in the inflows and outflows of river subbasins. Model output includes the spatial profiles of flow rates in a river section which occur as stream inflow, natural diffuse inflow, groundwater inflow, surface irrigation return flow, tributary inflow, and municipal-industrial effluent discharges. These flows are mixed in a stream segment and adjusted for evapotranspiration, system storage changes, and precipitation to arrive at the section outflows. The chemical phases of the model are based on computing monthly averages except if diurnal distribution of stream temperature and/or dissolved oxygen are requested.

INPUT REQUIREMENTS:

The model is divided into four submodels: (1) hydrology; (2) electrical conductivity; (3) temperature; and (4) dissolved oxygen. Attempts to model BOD and coliform counts were unsuccessful and not suggested for general application. A system control submodel is used to control the order of calculations, input data, and coordinate submodel interactions.

Inputs to the hydrology submodel consists of precipitation, measured stream inflows in the main channels, measured surface inputs, unmeasured surface and subsurface inflows, cropland diversions, reservoir storage, municipal-industrial diversions, pumped water, surface exports, and mean air temperature. The results from the hydrology submodel detail the flows within the river section. These flows are characterized by input electrical conductivities or flow versus electrical conductivity relationships. Simulation of stream temperature requires data describing the temperature of the respective inflows to a river section along with stream depth, discharge, and width to depth ratios to calculate heat equilibrium rates. The dissolved oxygen submodel requires that the initial oxygen level, BOD_{12} concentration, and rate constants be known. Flow data are supplied by other submodels.

SPATIAL AND TIME SCALES:

Although the model has the capacity for day to day change in stream temperatures and dissolved oxygen, the effective time resolution is one month. The scale encompasses major river segments in which uses and natural inputs tend to be lumped rather than distributed.

COMPUTER CODE STRUCTURE:

The program code is in the form of a single main program divided into segments by return controls and is coded in Fortran IV for a Univac 1108 computer. Core requirements listed are 20 k bytes of 32 bit words. Execution time is on the order of 30 seconds.

BASIC MATHEMATICAL APPROACH:

The hydrologic submodel is a mass balance simulation of the water flow along the stream segment. Precipitation falling on the land surface is routed through a snow melt equation when the seasonal transitions occur. Consumptive use is estimated with the Soil Conservation Service version of the Blaney-Criddle equation. The transport of water into and out of the groundwater is based on simple delay coefficients, and average storage values. This groundwater segment of the hydrologic submodel is actually evaluated by residual calculations by adjusting the delay coefficients until reasonable flows are predicted.

The basis of the salinity submodel is derived from functions relating discharge to salinity. Such expressions are developed for each flow segment used as input and then computed for the output values based on flow mixing.

Temperatures of the surface flows are predicted using linear regressions of air temperature and water temperature. Respective flows given as input are mixed to predict outflow temperatures. Some simulation is possible using sine functions of air temperature. The changes in water temperature inside a stream segment is based on a LaBouquet decay function.

The dissolved oxygen submodel utilizes the Streeter-Phelps oxygen sag equation. The BOD impact on dissolved oxygen is evaluated by the Hansen-Frankel equation. The first-order rate coefficients are taken from the literature.

GENERAL:

The reference cited above contains both a listing and a detail set of user instructions. The hydrology submodel has been substantially updated in other work at Utah State University.

MODEL: F-5

REFERENCES:

Hill, R.W., E.K. Israelsen, and J.P. Riley, 1973. Computer simulation of the hydrology and salinity system within the Bear River Basin. PRWG 104-1. Utah Water Research Laboratory, Utah State University, Logan, Utah. 122 pp.

Narasimhan, V.A., and E.K. Israelsen, 1975. A water-land use management model for the Sevier River Basin, Phases I and II. Information Bulletin 24. Utah Water Research Laboratory, Utah State University, Logan, Utah. September. 44 pp.

Huber, A.L., E.K. Israelsen, R.W. Hill, and J.P. Riley, 1976. Basin simulation assessment model documentation and users manual. PRWG 201-1. Utah Water Research Laboratory, Utah State University, Logan, Utah. August. 30 pp.

MODEL SCOPE:

Simulation involves the basic hydrologic relationships in river basins and/or watersheds. The model incorporates relationships describing hydrologic processes which are linked together by the conservation of mass principle. Salinity is added to simulation by assuming the hydrologic processes change the chemical concentration in the system by storing, concentrating, diluting and/or picking up salts. Salinity related processes are specifically developed for irrigated soils and small storage reservoirs.

The model concept is one of inflow-outflow = change in storage. Inflows simulated include stream inflows, tributary inflow, precipitation, subsurface inflow, and imports. Outputs are surface and subsurface flows, evaporation and evapotranspiration, and exports. Internal system simulations consider canal and groundwater diversions, surface and subsurface irrigation return flow, and soil moisture groundwater systems. Reservoir operations are provided with a specific submodel.

Use of this model falls under two categories. First, given the necessary input data, the simulation of various hydro-salinity flows is compared with actual measured values in order to calibrate the model. A pattern-search optimization technique is utilized to systematically optimize the calibration. The second model use which is based on proper calibration is to test management alternatives (changes in cropping patterns, alternative reservoir operations, and improved irrigation practices) on the water quality of the system outflows.

INPUT DATA:

Control parameters allow user to select one of four input options: (1) read run data for reduction and handling internally; (2) read data directly to simulation system; (3) read data from computer memory; and (4) read parameter bounds for calibration process. Other control parameters set boundaries for calibration process. Input of a hydrologic nature which must be supplied includes monthly percentage of daylight hours, crop and phreatophyte consumptive use coefficients, canal diversion, land use acreages, precipitation, soil moisture characteristics, temperature, river inflow, tributary inflow, subsurface inflow, surface outflow, and reservoir operations. Salinity data are also necessary for the above noted water flows.

SPATIAL AND TIME SCALES:

Simulation is of single or multiple river system subbasins. Analysis is partially dynamic in nature although steady-state is assumed within a time frame of 1 month. Time resolutions are monthly with multiple year analyses inherent. Model is two-dimensional in nature.

COMPUTER CODE STRUCTURE:

Internal program linkage is accomplished by subroutines with call and common data transfer. The program in its initial versions was written and utilized on a digital-electric analog hybrid computer at Utah State University. Hydrology is currently available in a digital format. The digital segments should be adaptable to other computer systems without much difficulty. Language is Fortran IV.

Execution time and memory requirements are not given. General examination indicates core requirements on the order of 50-70 k bytes and execution times on the order of 3-5 minutes for major calibration-simulation runs.

BASIC MATHEMATICAL APPROACH:

The basic mathematical relationship in the model is the conservation of mass within a river basin subarea:

$$(PPT + QSI + QGI) - (CET + QSO + QGO) = AS$$

where, PPT = precipitation
QSI = total surface inflow
QGI = total groundwater inflow
CET = evapotranspiration
QSO = total surface outflow
QGO = total groundwater outflow
AS = change in system storage in snow, soil moisture, surface reservoirs, and groundwater.

The principal model variable is QSO. As a generally known quantity, the model simulations of QSO are compared with measured values. Calibration involves adjusting various time lag and simulation coefficients until the error in the predicted values of QSO is minimal. The minimization approach has been termed a pattern-search technique which is essentially a process of iteratively varying the parameters to achieve minimum variance.

GENERAL:

This model is one of the most recent in a long-term program of hydrologic modeling at Utah State University. Many of the earlier models or versions thereof have been incorporated or omitted from this model based on applications in a number of field situations. A listing is included in the reference by Huber, et al. (1976).

MODEL: F-6

REFERENCES:

Walker, W.R. 1970. Hydrosalinity model of the Grand Valley. Unpublished M.S. Thesis, Civil Engineering Department, Colorado State University, Fort Collins, Colorado. August. 94 pp.

MODEL SCOPE:

This simulation is limited to the hydrologic and salinity systems in an irrigated valley. Diversions from reservoirs, rivers, tributary inflows, or groundwater are routed through the agricultural system. Surface as well as subsurface flows and flow qualities are predicted along with consumptive use.

INPUT REQUIREMENTS:

Input data consist of mean monthly values for temperature, percent daylight hours, Blaney-Criddle climatic coefficients, areas of each land use, Blaney-Criddle crop growth stage coefficients, river inflows, tributary inflows, river outflows, lateral diversions, surface drainage outflows, drainage base flows, soil moisture storage capacities, root zone diversions, exports, imports, water table fluctuations, precipitation, and equilibrium salinity concentrations of each of these flows. A series of groundwater data are also required. These include the number of strata at the groundwater basin's return flow point, and the number of normal locations where the gradient in each of these strata is defined. At the outflow point or close by, an initial value of hydraulic conductivity and cross-sectional area is required.

SPATIAL AND TIME SCALES:

The scale of the model is a macroscopic simulation of an irrigated area and the hydrology immediately surrounding it. A time resolution of one month is taken. Analysis is steady-state.

COMPUTER CODE STRUCTURE:

The computer code consists of a main program and subroutine served by both common and call statement data transfer. Written in Fortran IV, it should be adaptable in most computers. Core requirements are approximately 43 k bytes and time needs are about 25-30 central processor seconds per run.

BASIC MATHEMATICAL APPROACH:

A mass balance is made of the water flow system and the salt system is attached by multiplying by the concentrations associated with each segment of the system. Flows entering the main conveyance are segregated into seepage by a conveyance efficiency, lateral diversions as input, and operational wastes by difference. Lateral diversions are likewise delineated into seepage, root zone diversions, and tailwater. Finally, root zone diversions are allocated to root zone storage, deep percolation or consumptive use.

Summing the surface and subsurface flows from each breakdown yields an estimate of the respective return flows. At this point an estimate of the groundwater return flows is made on the basis of a groundwater model. A comparison of the mass balance and groundwater model estimates of subsurface return flows is made in a manner which calculates an adjusted aquifer hydraulic conductivity by month. The model is then systematically adjusted until the values of hydraulic conductivity are homogeneous. When the water system is satisfactorily modeled, the salinity system is added.

GENERAL:

The model is a second or third generation modeling concept initiated at Utah State University. Consequently, these early models will not be described; however, this model is an approach that can be applied with generally available data. The evapotranspiration and root zone analysis needs updating. Application has been made with good accuracy in the Grand Valley of western Colorado.